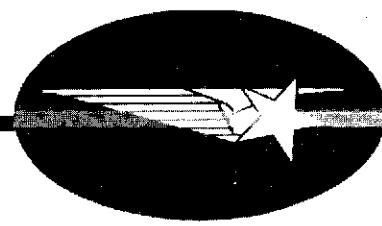


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STUDY OF HELIUM EMISSIONS
FROM ACTIVE SOLAR REGIONS

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by
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I

ABSTRACT

A theoretical study is made of the visible and UV line radiation of He I atoms and He II ions from a plane-parallel model flare layer. Codes have been developed for the solution of the statistically steady state equations for a 30 level He I - II - III model, and the line and continuum transport equations. These codes are described and documented in the report along with sample solutions. Optical depths and some line intensities are presented for a 1000 km thick layer. Solutions of the steady state equations are presented for electron temperatures 10^4 - 5×10^4 K and electron densities 10^{10} - 10^{14} cm⁻³.

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HELIUM EMISSION FROM ACTIVE SOLAR REGIONS

I. INTRODUCTION

The purpose of this program has been to develop codes for the simultaneous calculation of He I and II resonance line and He I D₃ line intensities from model flare regions. These lines were chosen because of the spectral ranges of the Skylab high resolution spectrographs and because of the planned program to obtain D₃ filtergrams on a patrol basis at the Lockheed Rye Canyon Observatory during the ATM mission. The NRL spectroheliograms incorporate simultaneous measurements of the He I and II resonance lines.

A plane-parallel layer irradiated on one side by the photospheric radiation field was chosen as the geometric model. A statistically steady state and uniform electron temperature and density with position were assumed. The energy level model consists of all terms through principal quantum number 4. Our study has been confined to conditions we believe characteristic of flare regions, namely electron temperatures between 10^4 and 5×10^4 °K and electron densities between 10^{10} and 10^{14} cm^{-3} . An extensive compilation of electron impact excitation rates has been made as part of this study. The results were published in Solar Physics (Benson and Kulander, 1972).

The statistically steady state level populations of model He I atoms have been calculated by a number of investigators for temperatures and densities characteristic of the outer solar atmosphere. Almost none of these authors has considered a sufficiently detailed energy level structure in the model atom to accurately obtain the D₃ line emission. Jefferies (1955) e.g. treats the 2s and 2p levels as a single level. De Jager and de Groot (1957) consider the 2s and 2p terms separately but the term structure of higher levels is ignored. This higher term structure is also ignored by Athay and Johnson (1960). They also neglect the effect of the He II ion processes by using other values for the

He I/He II equilibrium. Athay and Johnson arrive at the conclusion that in the temperature range $40,000 - 50,000^{\circ}\text{K}$, the D_3 line will appear in emission for $n_e \geq 10^{12}$ almost independently of T_e .

Zirin (1956) assumes in his calculations that transitions between terms of a given level are of negligible importance in determining the occupation numbers. This is known to be a poor assumption. Shklovsky and Kononovitch (1958) have calculated the D_3 line intensity but have made a number of unrealistic physical assumptions. More recently Hearn (1969) has calculated the occupation numbers of a 41 level He I atom and one level He II ion but he only presents results for the resonance line intensities. We shall demonstrate that more levels are required in He II to obtain correct line intensities.

Jefferies (1957) has calculated the D_3 line intensity from a layer assumed to be optically thick in the D_3 line. The transport equation was solved assuming incoherent scattering with no photospheric radiation in the line. Jefferies' results are very qualitative since it is known that the D_3 line is probably not optically thick.

To obtain accurate line intensities, simultaneous solution of the line and continuum radiative transfer equations and the steady state populations is required. To accomplish this, we have developed three separate codes. The first code (Code 1) solves the statistical equilibrium equations for a 30 level He I-II-III system given the appropriate rates. The basic equations and sample solutions are given in Section II. The code is described in Section V and a listing is given in Appendix A.

The second code (Code 2) represents a numerical solution of the line transport equations for a finite layer. The solution is of the integral form of the transport equation by expansion of the source function in terms of a finite sum. The mathematical method used is summarized by Avrett and Loeser (1969). Complete frequency redistribution and a Gaussian absorption profile are assumed. The basic equations and sample

solution are given in Section III. The code is described in Section V and a listing is given in Appendix B.

The third code (Code 3) solves the continuum transport equation by expansion of the source function in a very similar manner to the line transport equation. The equations are given in Section IV. The code is described in Section V and a listing is given in Appendix C.

III. THE STEADY STATE EQUATIONS

A. Energy Level Model

The 30 assumed energy levels for the system of ions He I - He III are given in Table II-1. There are 19 levels for He I, 10 for He II and 1 for He III. These levels are shown in Figures II-1 and II-2. The levels are numbered 1 - 30 in order of increasing energy. Levels 1, 20 and 30 are the ground states of He I, II and III, respectively. This model was chosen to provide accurate solution for the first two resonance lines in He I and II and the D₃ and 10830 lines of He I. Many other lines are included but were not the primary lines under consideration. The allowed transitions included in the model are listed in Table II.2 together with f numbers and wavelengths. The inclusion of the 4 S, P, D and F levels separately is necessary because at the lower electron densities considered radiative de-excitation rates can become larger than collision rates between the n = 4 levels. At higher electron densities the collision rates between the n = 4 terms dominate all other rates in or out of these terms and the relative populations are Boltzmann.

B. Population Equations

The rate equation describing the population of the bound or continuum state i is

$$S_{\gamma j} \left(R_{\gamma ji} - R_{\gamma ij} \right) = 0 \quad \text{III.1}$$

where $R_{\gamma ji}$ and $R_{\gamma ij}$ are the total transition rates/cm³ by process γ from state j to i and from i to j respectively. The sum S represents a sum over discrete states and an integration over continuum states. We shall assume the particle translational distribution functions to be Maxwellian and the external continuum radiation field to be Planckian, in which case it is possible to integrate over the continuum and replace it by one additional term in the discrete sum. The atomic transition processes are radiative excitation and ionization, collisional excitation and ionization by atoms and electrons and their inverses. Because of their higher velocities, electron collisions generally dominate the collisional rates and hence only electron inelastic rates will be considered.

TABLE II.1
He I, II Energy Levels

He I - i = 1

j			Energy (ev)	Wave Nos.	St. Wt.
1	$1s^2$	1S	0	0	1
2	$1s2s$	3S	19.821	159850	3
3	$1s2s$	1S	20.618	166272	1
4	$1s2p$	$^3P^0$	20.966	169081	9
5	$1s2p$	$^1P^0$	21.220	171129	3
6	$1s3s$	3S	22.721	183231	3
7	$1s3s$	1S	22.923	184859	1
8	$1s3p$	$^3P^0$	23.009	185559	9
9	$1s3d$	3D	23.076	186096	15
10	$1s3d$	1D	23.076	186099	5
11	$1s3p$	$^1P^0$	23.089	186204	3
12	$1s4s$	3S	23.596	190292	3
13	$1s4s$	1S	23.676	190935	1
14	$1s4p$	$^3P^0$	23.710	191211	9
15	$1s4d$	3D	23.738	191439	15
16	$1s4d$	1D	23.739	191441	5
17	$1s4f$	$^3F^0$	23.739	191447	27
18	$1s4f$	$^1F^0$	23.739	191447	7
19	$1s4p$	$^1P^0$	23.744	191487	3

He II - i = 2

1	$1s$	2S	0	0	2
2	$2s$	2S	40.8099	329179.57	2
3	$2p$	$^2P^0$	40.8091	329182.02	6
4	$3s$	2S	48.3662	390140.76	2
5	$3p$	$^2P^0$	48.3664	390141.49	6
6	$3d$	2D	48.3665	390142.64	10
7	$4s$	2S	51.0113	411476.98	2
8	$4p$	$^2P^0$	51.0114	411477.28	6
9	$4d$	2D	51.0115	411477.77	10
10	$4f$	$^2F^0$	51.0117	411477.95	14

TABLE II.2

He I, II Lines

He I

Upper Level	Lower Level	Notation	$\lambda(\text{\AA})$	A ($10^8/\text{sec}$)	f
4	2	1	10830	.1022	.5391
5	1	2 UV	584.4	17.99	.2762
5	3		20582	.01976	.3764
6	4	10	7065	.278	.0693
7	5	45	7281	.181	.0480
8	2	2	3889	.09478	.06446
8	6		4.30+4	.0108	.896
D3 →	9	11	5876	.706	.609
	9		1.86+5	1.28-4	.111
	10	46	6678	.638	.711
	11	3 UV	537.1	5.66	.0734
	11	4	5016	.1338	.1514
	11		7.43+4	.00253	.629
	12	12	4713	.106	.0118
	12		21120	.0652	.145
	13	47	5049	.0655	.00834
	13		21132	.0459	.103
	14	3	3188	.0505	.0231
	14		12538	.00608	.0429
	14		19543	.00597	.0205
	14		1.09+5	.0505	1.21
	15	14	4472	.251	.125
	15		17002	.0668	.482
	15		4.39+5	4.16-5	.200
	16	48	4922	.202	.122
	16		19089	.0711	.647
	17		18688	.139	1.02
	17		1.43+7	6.01-10	.0033
	18		18699	.138	1.01
	18		1.67+7	4.34-10	.00253
	19	4 UV	522.2	2.46	.030
	19	5	3965	.0717	.0507
	19		15088	.0137	.140

TABLE II.2 (Continued)

He I

Upper Level	Lower Level	Notation	$\lambda(\text{\AA})$	A ($10^8/\text{sec}$)	f
19	10		18560	.00277	.00858
19	13		1.81+5	5.78-4	.853
19	16		2.17+6	5.65-7	.024

He II

3	1		303.80	100.	.4162
4	3		1640.5	1.01	.01359
5	1		256.3	26.8	.07910
5	2		1640.4	3.59	.4349
6	3		1640.4	10.3	.6958
7	3		1215.1	.413	3.045-3
7	5		4687.0	.294	.03225
8	1		243.03	10.9	.02899
8	2		1215.1	1.55	.1028
8	4		4686.8	.491	.4847
8	6		4687.2	.056	.01099
9	3		1215.1	3.30	.1218
9	5		4686.9	1.13	.6183
10	6		4687.1	2.21	1.018

Fig. II-1 ENERGY LEVEL DIAGRAM FOR IDEALIZED HeI ATOM

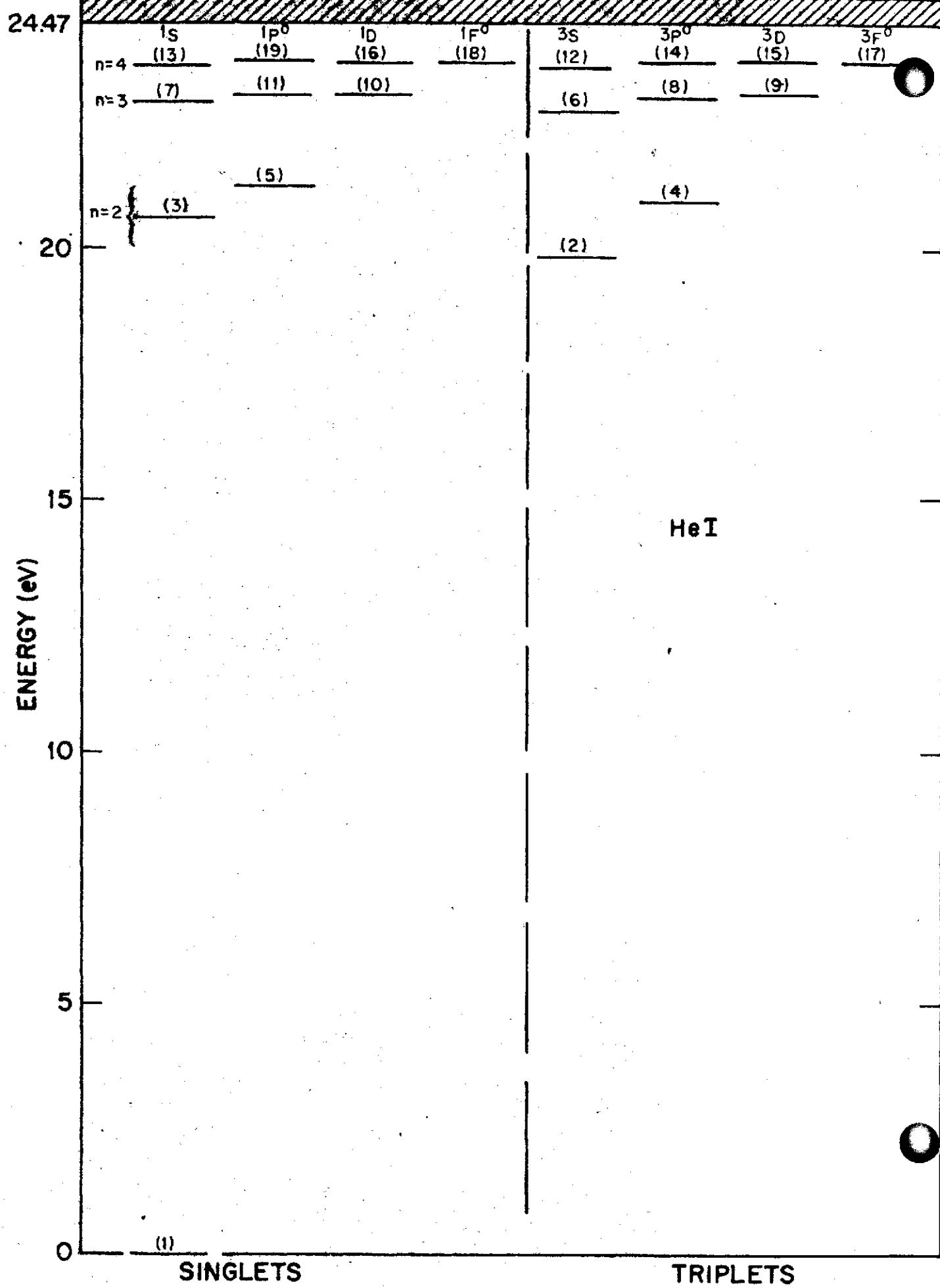
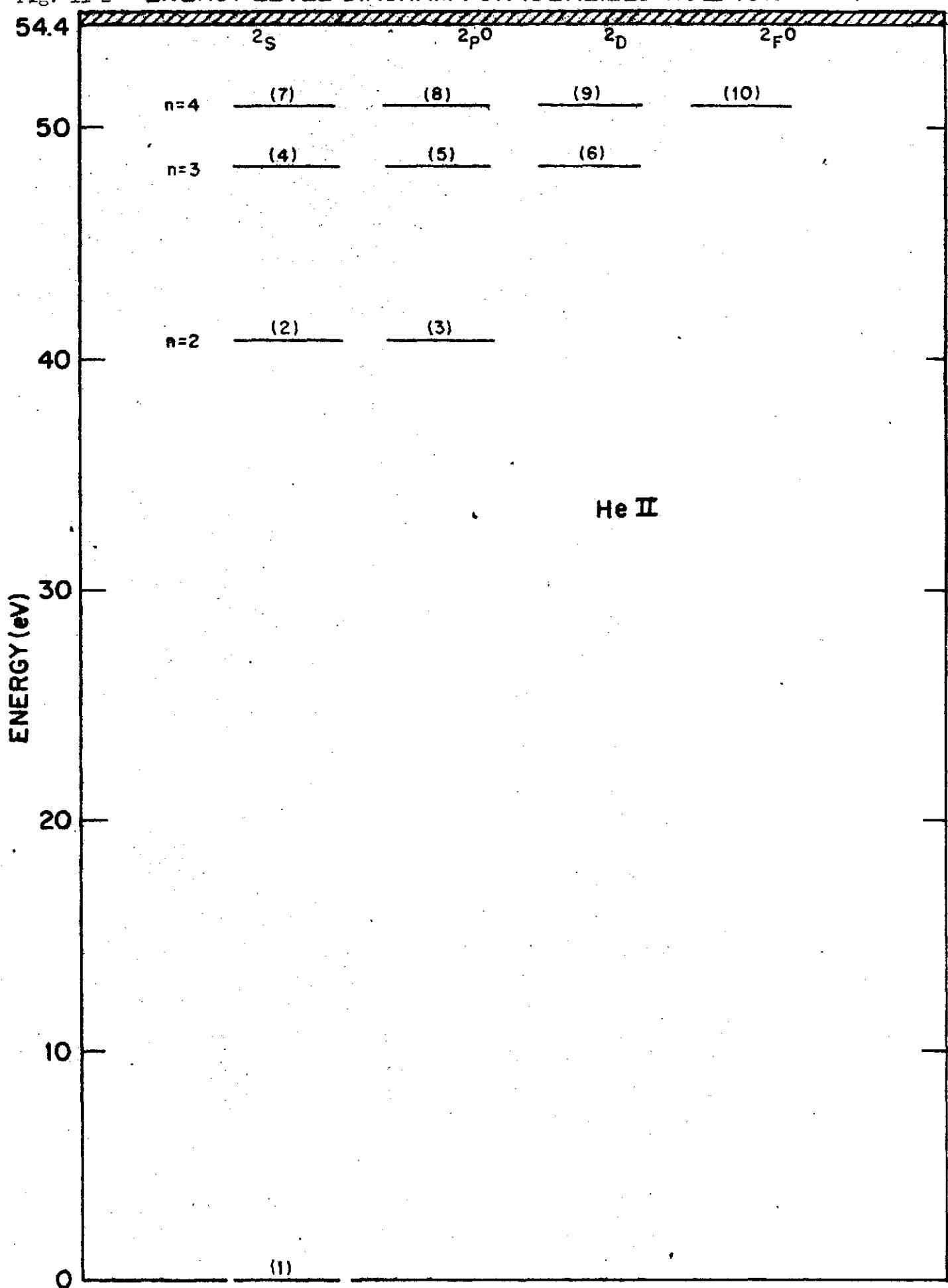


Fig. II-2 ENERGY LEVEL DIAGRAM FOR IDEALIZED He II ION

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We may write the total rate from i to j more specifically as,

$$R_{yij} = n_i P_{ij} = n_i (A'_{ij} + C_{ij}), \quad \text{III.2}$$

where A'_{ij} and C_{ij} are the radiative and collisional transition rates/particle from the ith to the jth state. In the statistically steady state, equation III.1 reduces to

$$\sum_{j \neq i} (n_j P_{ji} - n_i P_{ij}) = \sum_j n_j P_{ji} = 0; \quad P_{ii} = -\sum_{j \neq i} P_{ij}. \quad \text{III.3}$$

The system of equations represented by III.3 can easily be solved for the populations n_i when all the P_{ij} 's are known. This is the case when the gas is totally optically thin (in all lines), since the external radiation field is specified and the internal radiation field does not produce a significant upward transition rate. We can characterize the system of linear equations (III.3) by a matrix whose coefficients a_{ij} are equal to P_{ji} . The diagonal elements are the P_{ii} .

The general solution of equations (III.3) is given by White (1961)

$$n_i = \lambda_m P^{mi}; \quad \lambda_m = \frac{N}{\sum_i P^{mi}}, \quad \text{III.4}$$

where P^{mj} is the co-factor of the coefficient of n_j in the mth equation (i.e. the matrix element P_{mj}) and N is the total number of He particles/cm³. We denote the discrete level corresponding to the continuum, i.e. an ionization or recombination, by c. We may then write the rate equation for level i of ion q as,

$$-(\sum_j P_{ij}^q + \sum_{j'} P_{icj'}^q + \sum_{j'} P_{cij'}^q) n_i^q + \sum_{j'} P_{j'i}^{c,q+1} n_{j'}^{q+1} + \sum_{j'} P_{j'i}^{q-1,c} n_{j'}^{q-1} + \sum_j P_{ji}^q n_j^q = 0 \quad \text{III.5}$$

where j and j' refer to other bound levels in the qth ion and in other stages of ionization, respectively, P_{ijl}^q is the total excitation or de-excitation rate in ion q from i-j; $P_{icj'}^q$ and $P_{j'i}^{q-1,c}$ are the total ionization rates from i in q to j' in q + 1 and to i in q from j' in q - 1, respectively; $P_{cij'}^q$ and

$p_{j'i}^{c,q+1}$ are the total recombination rates from i in q to j' in $q+1$ and to i in q from j' in $q+1$, respectively. Specifically we may write the P 's as follows:

bound-bound

$$i > j \quad P_{ij}^q = A_{ij}^q + Y_{ij}^q B_{ij}^q B_r + n_e \bar{\Omega}_{ij}^q \quad \text{II.6}$$

$$i < j \quad P_{ij}^q = Y_{ij}^q B_{ij}^q B_r + n_e \bar{\Omega}_{ij}^q$$

bound-free (from initial state q, i)

$$\text{ionization} \quad P_{icj'}^q = W \bar{A}_{ij'}^q + n_e \bar{\Omega}_{ij'}^q \quad \text{II.7}$$

$$\text{recombination} \quad P_{cij'}^q = n_e \alpha_{ij'}^q + n_e W \beta_{ij'}^q + n_e \bar{\Omega}_{ij'}^q$$

bound-free (to initial state q, i)

$$\text{ionization} \quad P_{j'i}^{q-1,c} = W \bar{A}_{j'i}^{q-1} + n_e \bar{\Omega}_{j'i}^{q-1} \quad \text{II.8}$$

$$\text{recombination} \quad P_{j'i}^{c,q+1} = n_e \alpha_{j'i}^{q+1} + n_e W \beta_{j'i}^{q+1} + n_e \bar{\Omega}_{j'i}^{q+1}$$

where n_e is the electron density/cm³; B_r is the Planck function at temperature T_r ; W is the dilution factor; Y_{ij}^q is a free parameter, A_{ij}^q , B_{ij}^q are the Einstein transition probabilities; \bar{A}_{ij}^q is the photoionization rate/ion; Ω_{ij}^q , $\bar{\Omega}_{ij}^q$ are the collisional transition rates/electron per ion for bound-bound and bound-free processes, respectively; $\bar{\Omega}_{ij}^q$ is the collisional transition rate/electron² per ion for free-bound recombination; and α_{ij}^q , β_{ij}^q are the recombination, and stimulated recombination coefficients, respectively.

The basic quantities required for the evaluation of the radiative rates are the oscillator strengths and photoionization cross sections; for the collisional rates the excitation and ionization cross sections. The inverse cross sections and Einstein coefficients can be obtained from the usual detailed balance relations. The quantities Ω , $\bar{\Omega}$, $\bar{\Omega}$ and α generally have the form

$$\int v Q(v) f(v) dv,$$

II.9

where v is the electron velocity, $Q(v)$ the cross section and $f(v)$ the electron translational distribution function. \bar{A} may be written in terms of the photo-ionization cross section $a(v)$ as

$$4\pi \int \frac{a(v)}{hv} B(v) dv. \quad \text{II.10}$$

β is expressed similarly in terms of the stimulated recombination cross section $b(v)$.

Solutions can be obtained for any arbitrary line radiation field by suitable choice of the parameter Y which is closely related to the net radiative bracket (NRB). Y varies between 0 and 1 being 0 for a thin layer (no external radiation) and 1 for a very thick layer where the line radiation field is Planckian. For a thin line with external photospheric radiation $Y = 1/2 B(T_e)$. Various continuum radiation fields can be considered by suitable choices of \bar{A} .

C. Reaction Rates

Oscillator strengths for all of the allowed transitions included in our model (Section II.A) were found in the NBS compilation by Wiese et al. (1966). Photoionization rates were obtained from Hartree-Fock calculations of Stewart and Webb (1963) for the ground state of He I and from calculations by Peach (1967) for the $n^1 S$, $n^3 S$, $n^1 P$ and $n^3 P$ levels. For all other levels cross sections were calculated using the quantum-defect method of Burgess and Seaton (1960).

Collisional ionization rates were obtained from measurements of Englander-Golden and Rapp quoted by Kieffer and Dunn (1966) for $1^1 S$, from measurements of Long (1967) for $2^3 S$ and from calculations of Dolder, et al. (1961) for the He II ground state. For other levels the ionization rates were taken from Allen (1961).

The collisional excitation cross sections are crucial to the solution of the steady state equations. For this reason we have made an extensive tabulation and study of rates from many sources. A paper entitled "Electron Impact Excitation Rates for Helium" describing these rates was published in the December 1972 issue of Solar Physics (Benson and Kulander, 1972). Excitation rates were calculated from most available cross section data, and fitted to the empirical formula

$$\Omega = AT^n \exp(-\alpha X_0)$$

where $X_0 = E_0/kT$; A , n and α are constants. For He I the temperature range considered was 4000-50,000°K and for He II, $10^4 - 10^5$ °K. Rates between all levels of the model of Section II.A were calculated. The inverse rates for both radiative and collisional transitions were calculated from standard equilibrium relationships.

We shall discuss briefly some of our conclusions concerning the electron impact rates beginning with the He I rates.

Generally both forbidden and allowed rates are in better agreement for higher temperatures than for lower temperatures. The allowed rates are in much better agreement than the forbidden rates. The allowed rates from ground state or level 2 generally show differences as large as a factor of 10 for low temperatures and as large as 5 for high temperatures. Between other levels ($n \geq 3$) the differences are only as much as factors of 3 at low temperatures and 50-100% at high temperatures.

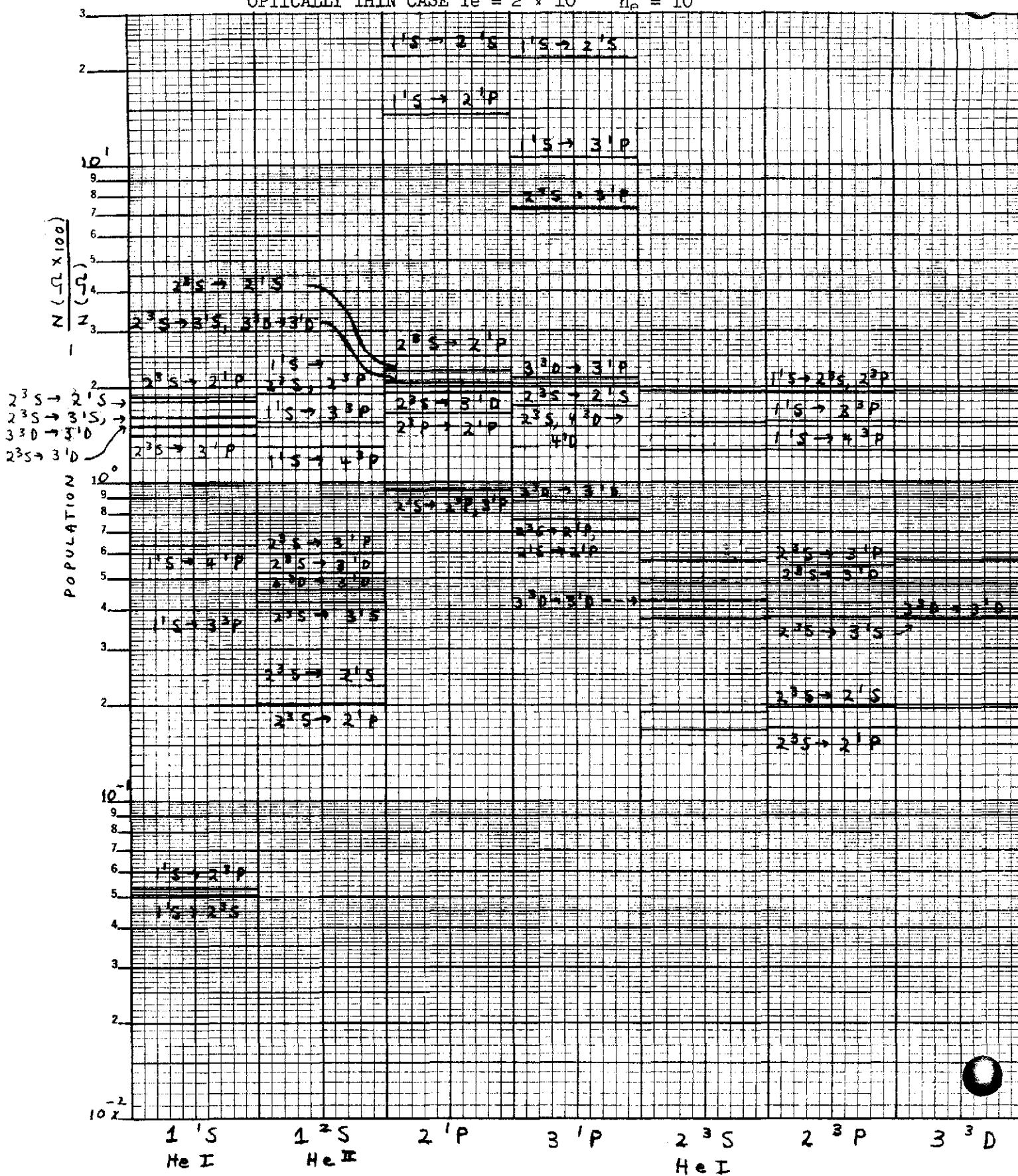
In He I the forbidden rates generally differ by as much as a factor of 100 at low temperatures, a factor of 20-50 at higher temperatures. Differences as high as a factor of 10^5 are noted in a few cases, differences of factors of 10^3 are not uncommon. If one does not consider the highest and the lowest rate value for each transition the differences are generally reduced to factors of about 10 at lower temperatures and 5 at higher temperatures. Forbidden transitions with lower level $n = 2$ show differences 2-3 times less than those with $n = 1$.

For transitions between the higher levels only the very approximate cross sections of Green (1966) and Allen (1963) are available for forbidden transitions and for allowed transitions those of Seaton (1962), Saraph (1964) and Mihalas and Stone (1968). Comparing the two approximate results for forbidden transitions with the other measured and calculated values we find the approximate results generally lower by factors of 2-10. For higher levels the Green cross sections are generally higher than those of Allen. With regard to the Seaton and Saraph approximations, it is not conclusive which is more often closer to the other values. The Seaton approximation gives values generally higher than the Saraph approximation for lower temperatures while the reverse situation holds for higher temperatures.

For He II there are relatively few cross sections available. The largest differences, being about a factor of 5, are much less than for He I. For both He I and He II experimentally determined cross sections give lower rates than the calculated values.

The actual collisional excitation rates chosen represent mean values of those given in the paper, taken from various sources listed there. To determine the sensitivity of the solution to these rates the statistical equilibrium equations were solved after increasing the individual values of the collision rates per electron Ω between each state by a factor of 100. This was done to determine the sensitivity of the solution to the collision excitation rates. We chose the optically thin case with $T = 20,000^{\circ}\text{K}$, $n_e = 10^{10}$ for this test. We illustrate in Figure II.3 the effect on the population of the levels 1, 2, 4, 9, 11 and 20 of each perturbation in collision rate. Of course in many instances increasing a particular Ω_{ij} by 100 had little effect on the populations of the levels mentioned. In Figure II.3 we show the 10 transitions $i-j$ which have the largest effect on each of the above levels. The ratio of the population after increasing Ω_{ij} by 100 to that before the perturbation is shown. We note that changes of 10 to 50 in these important populations result from an uncertainty of a factor of 100 in the rates.

All the triplet levels of He I had about the same response to the change in Ω . When the rate from the He I ground state (G.S.) to triplet levels increased the triplet populations increased. When the triplet to singlet rates increased the triplet populations decreased as would be expected. The He I G.S. population is very sensitive to the rate from the G.S. to the metastable $2\ ^3\text{S}$ level (and $2\ ^3\text{P}$ level). The $1\ ^1\text{S}$ level population was decreased by about 20 when $\Omega(1\ ^1\text{S} \rightarrow 2\ ^3\text{S})$ was increased by 100. At the same time the He II G.S. population was increased. An increased rate from the triplets to singlets results in increased $1\ ^1\text{S}$ population and a corresponding decrease in $1\ ^2\text{S}$ population. The populations of the upper levels of the 584 and 537 Å lines are very sensitive to the rate from the $1\ ^1\text{S}$ to $2\ ^1\text{S}$ level increasing as this rate increases.

Figure II-3 POPULATION CHANGE BY INCREASING Ω BY 100OPTICALLY THIN CASE $T_e = 2 \times 10^4$ $n_e = 10^{10}$ 

D. Sample Solutions.

A code which we shall designate as code 1 has been developed to solve the steady state population equations given in Section II.B. This code is described in Section V. We discuss in this section some sample solutions of the steady state population equations.

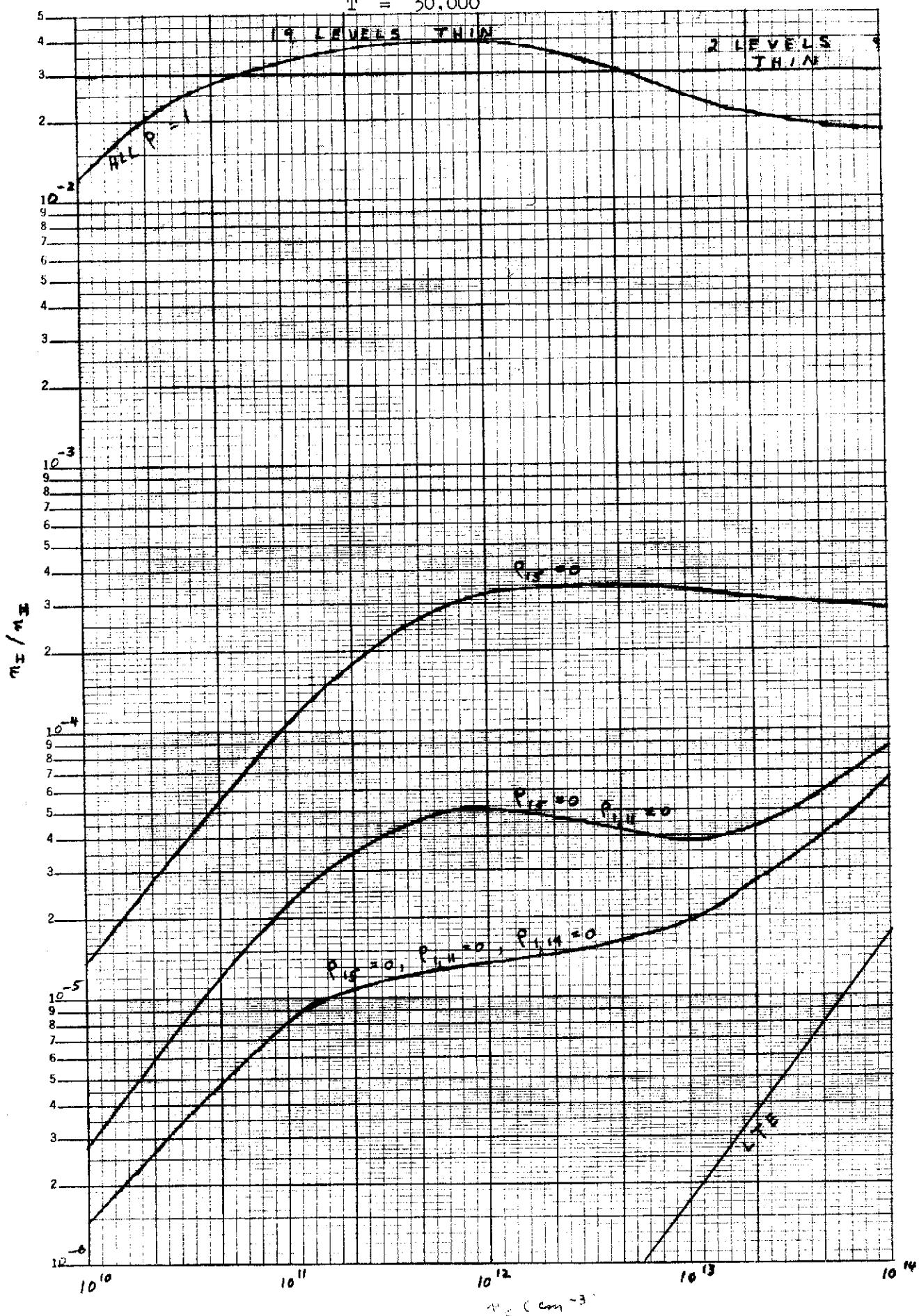
The gas is assumed irradiated over 2π ster by a Blackbody spectrum at 6000°K representing the photospheric radiation field. The gas is assumed to be optically thin for all lines and continua unless otherwise specified.

1. Ionization Equilibrium

In this section we illustrate results for the ionization equilibrium. Fig. II-4 shows the ratio n_1/n_{20} with $T_e = 30,000^{\circ}\text{K}$ at various values of n_e . For an atomic model with only levels 1 and 20 the ratio n_1/n_{20} is approximately constant with n_e since both the collisional ionization and recombination rates are proportional to n_e . The optically thin solution for two levels is shown. The results are generally within a factor of 2. For very low n_e , all of the levels of He I except 5, 11 and 19 represent additional paths from level 1 to level 20. This is so because the photoionization rates from these levels exceed almost all collisional rates. n_1/n_{20} is hence lower at $n_e = 10^{10}$ than the two level solution. For somewhat higher electron densities the collisional rates between the singlets and triplets exceed the photoionization rates. Hence, the recombination to intermediate levels results in conversion to the 5, 11 or 19 level and thence to the 1 level by spontaneous emission. The rate from 20 to 1 is now enhanced and n_1/n_{20} exceeds the two level solution. At still higher electron density the collisional ionization rates begin to become greater than either the spontaneous emission or collisional deexcitation rates. Now all intermediate levels represent paths from level 1 to 20 and n_1/n_{20} becomes lower than the two level solution. This is seen to be the case at $n_e = 10^{14}$.

We turn to the solution when the resonance lines are optically thick. The result for detailed balance (db) in the first resonance line is shown

Figure II-4 HELIUM IONIZATION EQUILIBRIUM

 $T = 30,000$ 

by the curve labeled $\rho_{15} = 0$ (ρ is the net radiative brackett). Also shown are results for db in the second and third resonance lines. Increasing the radiative excitation rate increases the effective ionization rate and the amount of n_{20} by several orders of magnitude. We thus note the important result that the ionization equilibrium is strongly influenced by the optical thickness of the resonance lines. The LTE result is also shown and is labeled LTE.

2. Level Populations

Many sample solutions have been obtained for the level populations or non-equilibrium parameters, b , where $b = n/n_{\text{equil}}$.

We have completed a parametric study of the effect of optical thickness in the resonance lines and continua upon the level populations. Level populations were obtained for various physically meaningful combinations of resonance lines and continua being optically thick or thin. That is to say each resonance line or continua was assumed to have a net radiative brackett of either 0 (completely thick) or 1 (thin). The results cover the temperature range $T = 10,000$ to $50,000^{\circ}\text{K}$ and electron density range $n_e = 10^{10} - 10^{14} \text{ cm}^{-3}$. Due to space limitations we cannot present results for all 30 levels of the model. Hence levels 1, 5, 9, 20 and 27 were chosen to illustrate the results. Referring to section II.A we see that levels 1 and 20 are the ground states of He I and II, level 5 the upper level of the 584\AA line, level 9 the upper level of the D₃ line and level 27 the upper level of the 4686\AA line of He II. Figures II.5-29 show results for each of these 5 levels for electron temperatures 10^4 , 2×10^4 , 3×10^4 , 4×10^4 and 5×10^4 K. In each figure the ratio of the actual population to the equilibrium population, b , is given as a function of n_e .

At each temperature calculations were made for combinations of net radiative brackets corresponding to layers of varying total thickness. There are 3 resonance lines in the model for both He I and He II. These 6 lines together with the Lyman continua for each ion are allowed to become optically thick in our calculation. Thus, there are eight lines and continua which can be optically thick or thin depending upon the physical thickness of the layer. Each figure shows a completely optically thin solution labeled T and 8 other solutions labeled 1 - 8 which correspond to the combinations of optical

Figure II-5 b_1

$$T_e = 10,000^{\circ}K$$

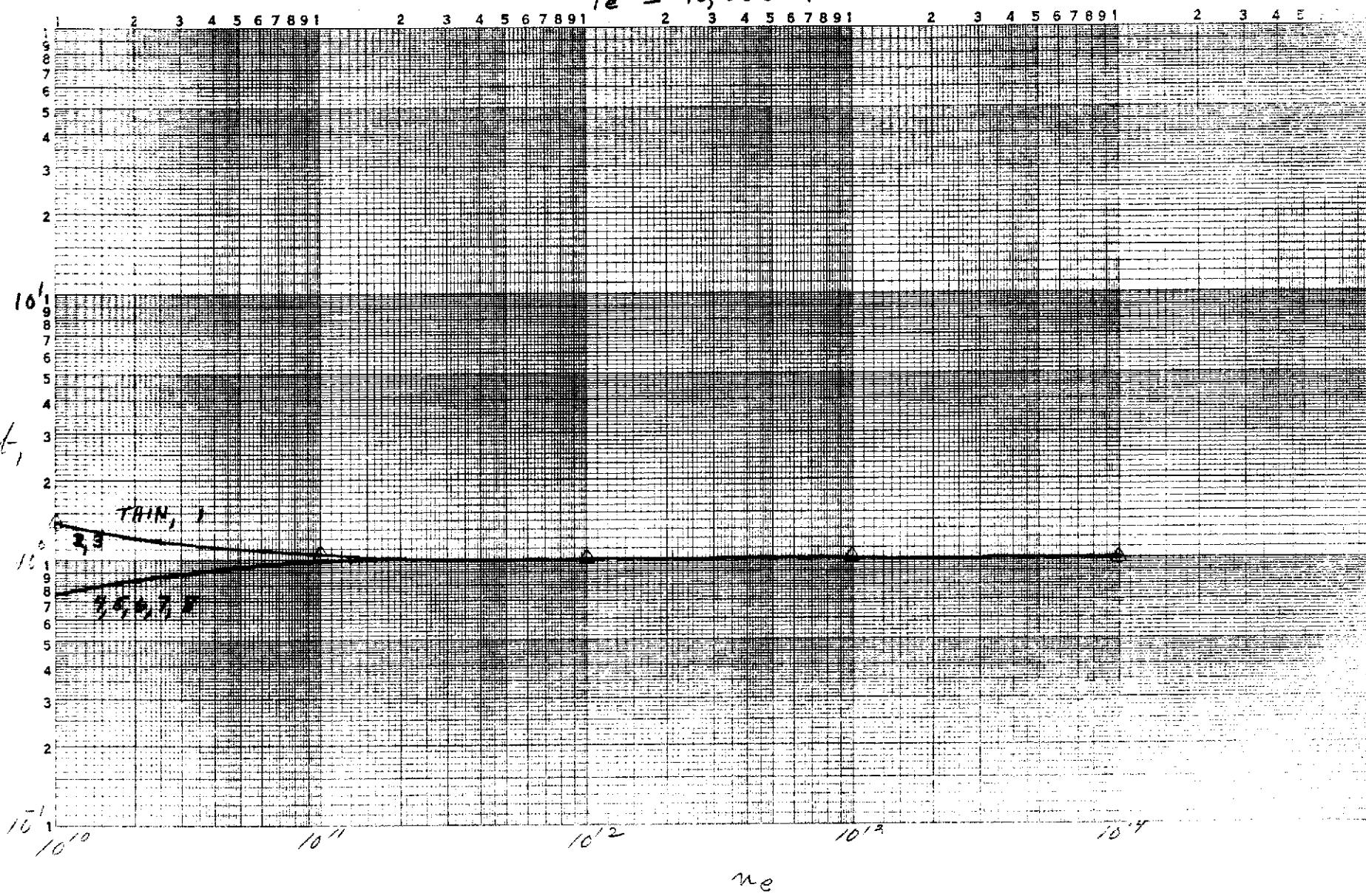


Figure II-6 b₉

$$T_e = 10,000^\circ K$$

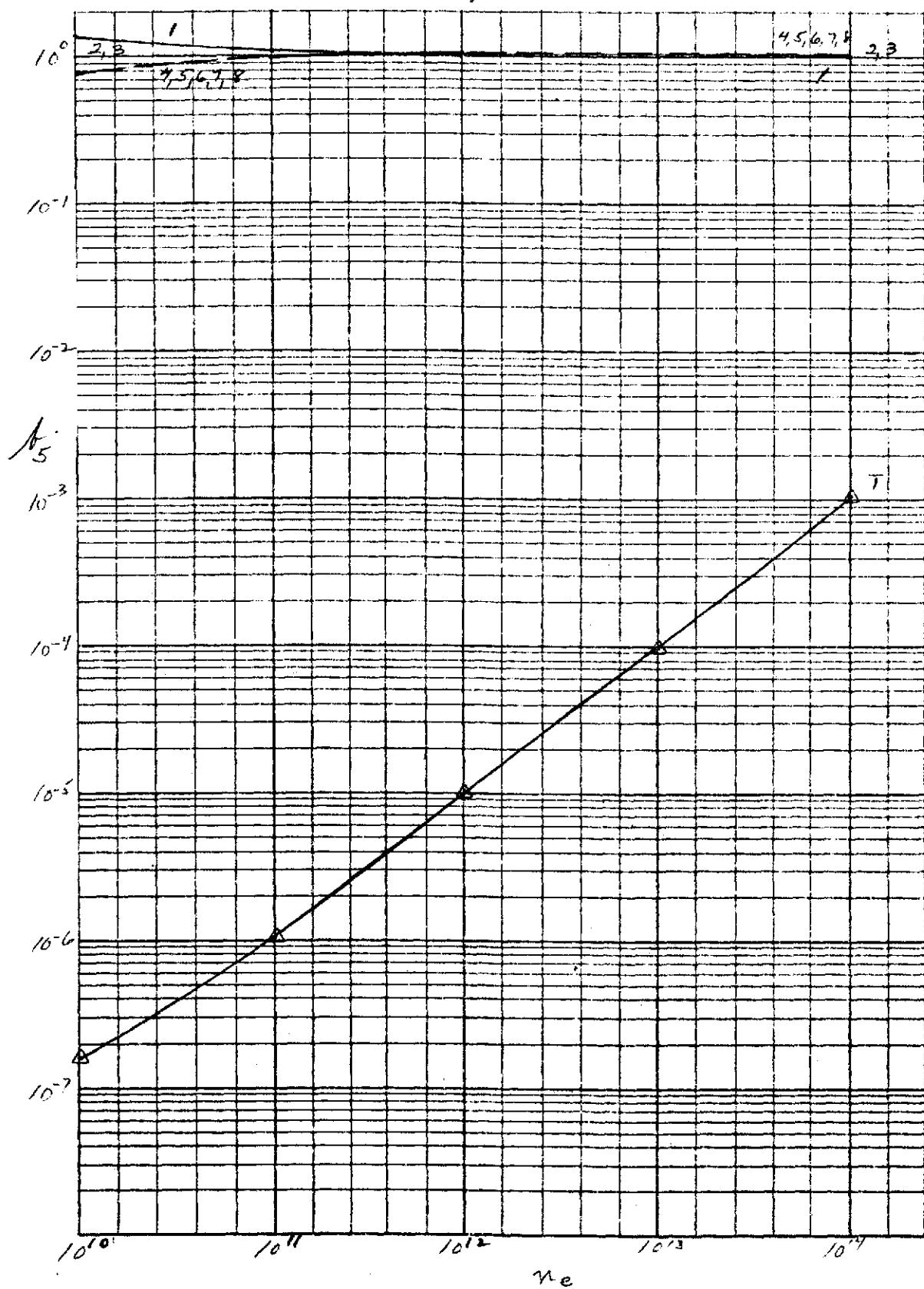


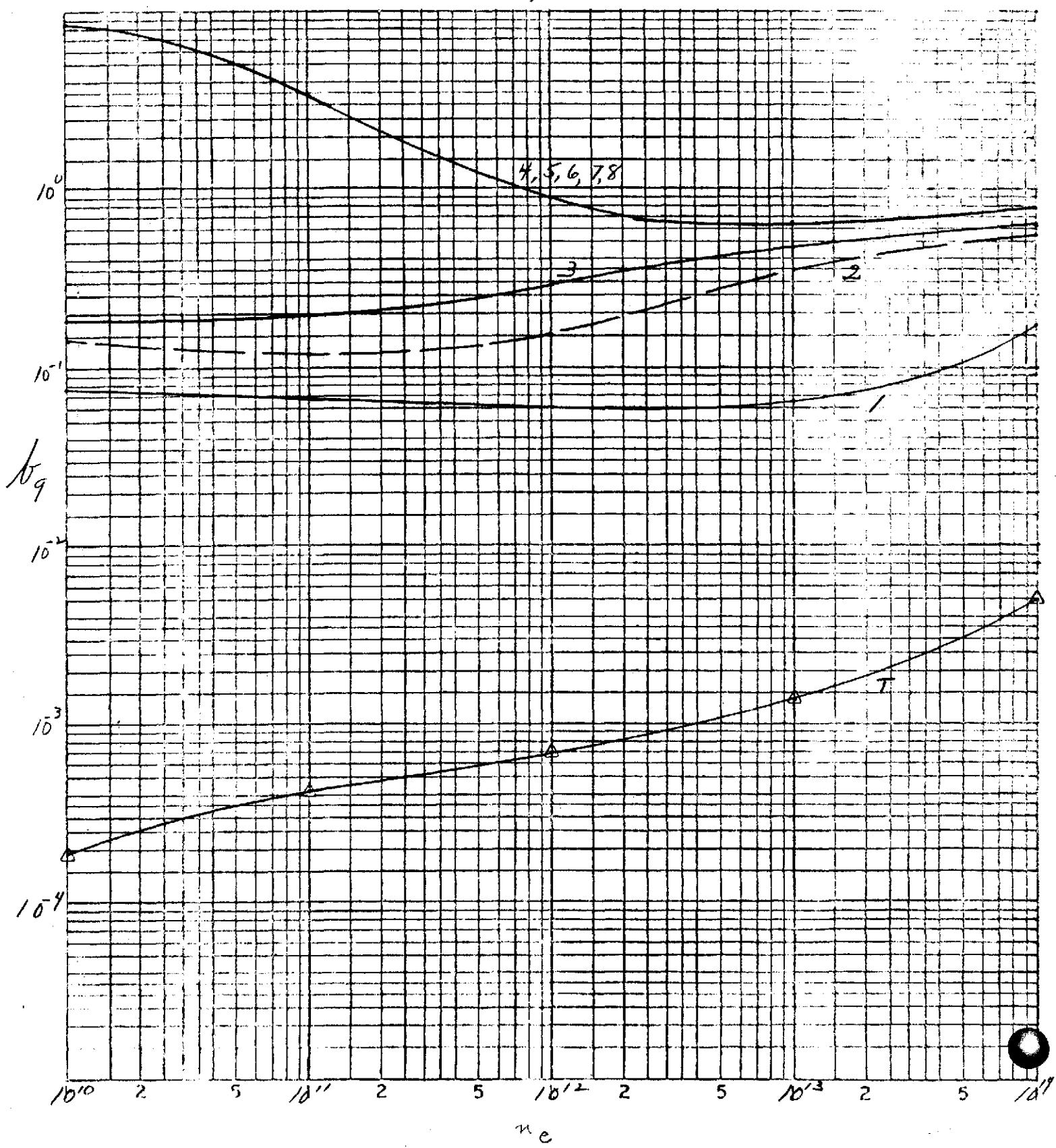
Figure II-7 b_9 $T_e = 10,000^\circ K$ 

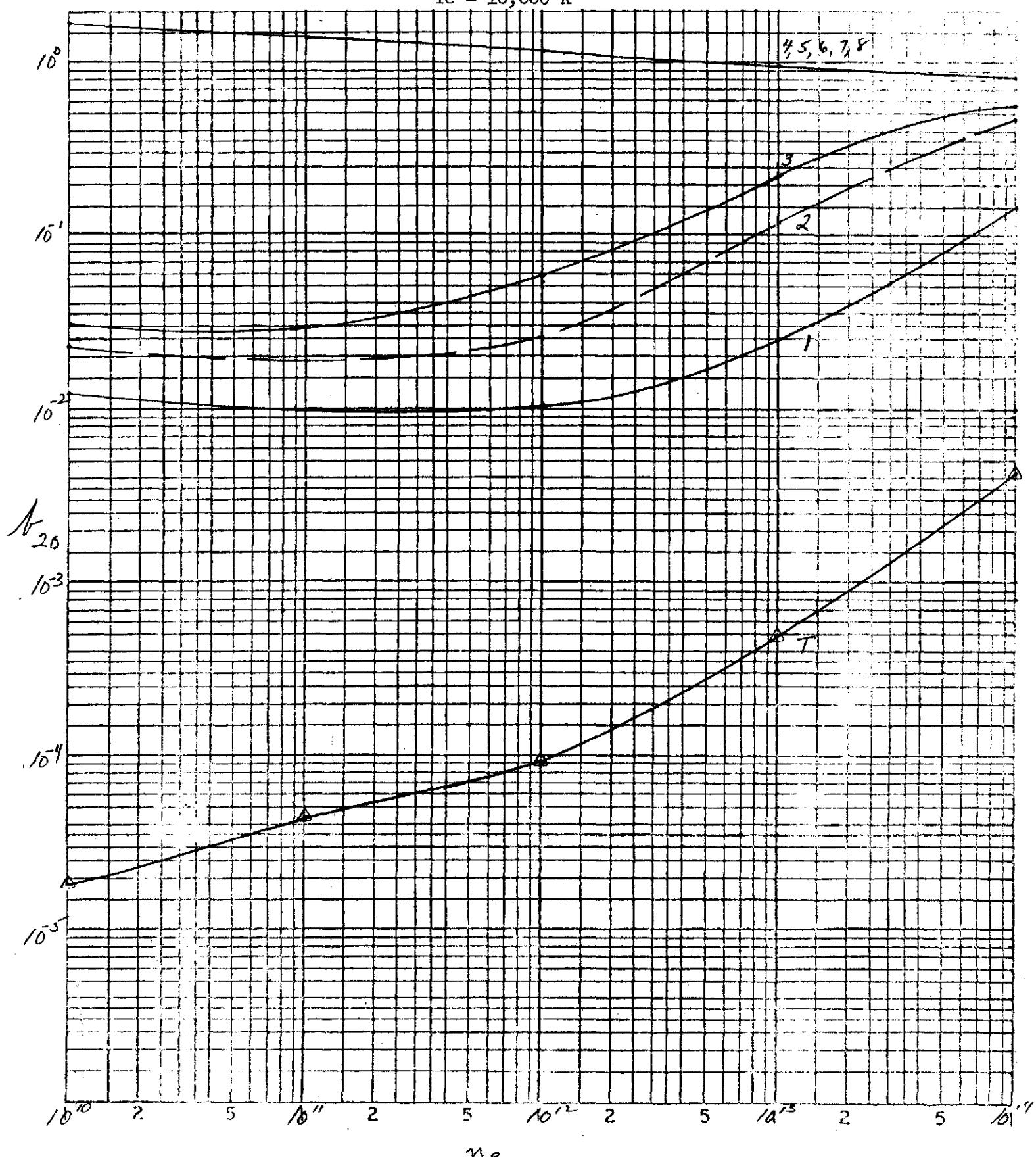
Figure II-8 b_{20} $T_e = 10,000^\circ K$ 

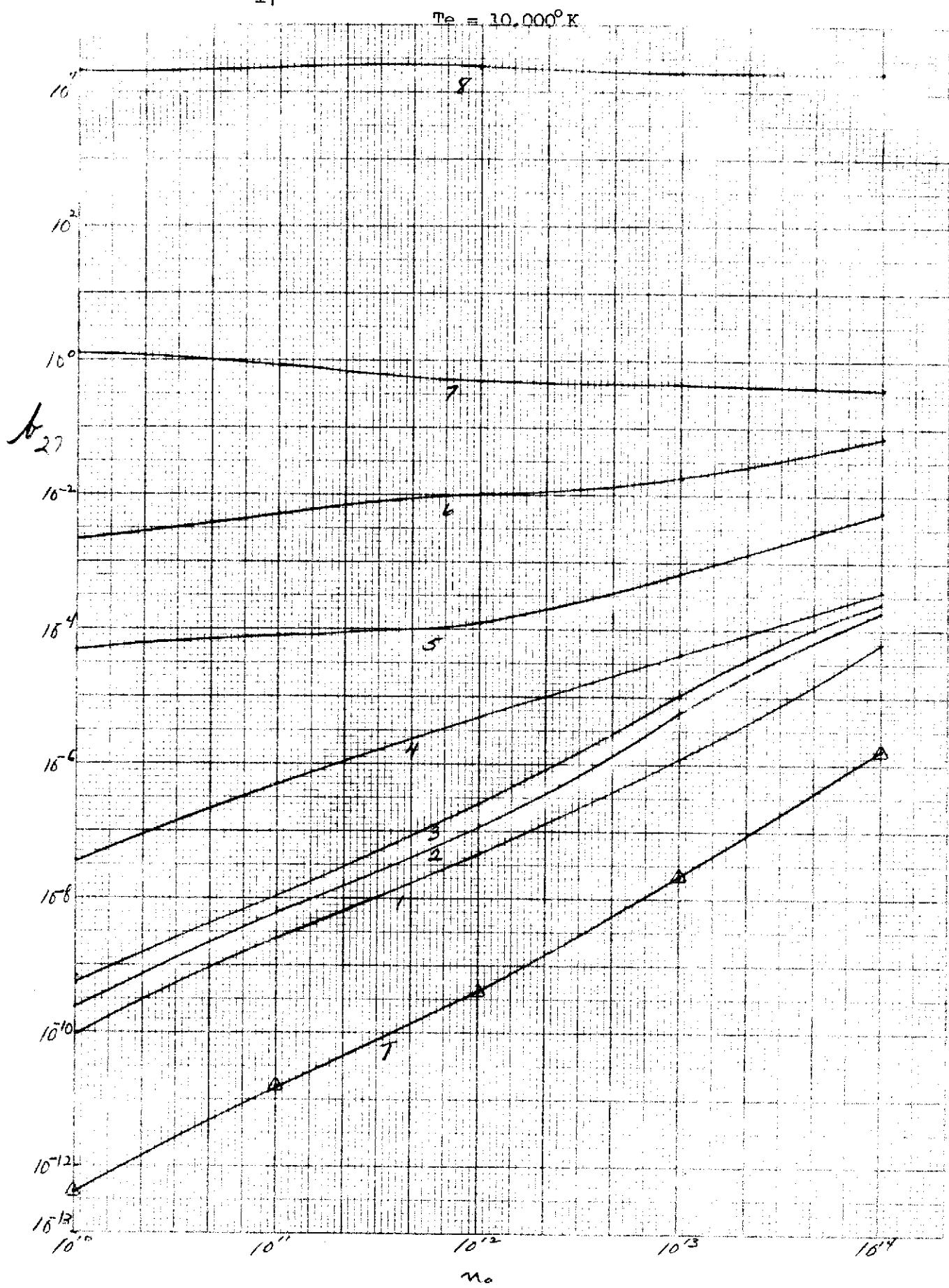
Figure II-9 b₁₇

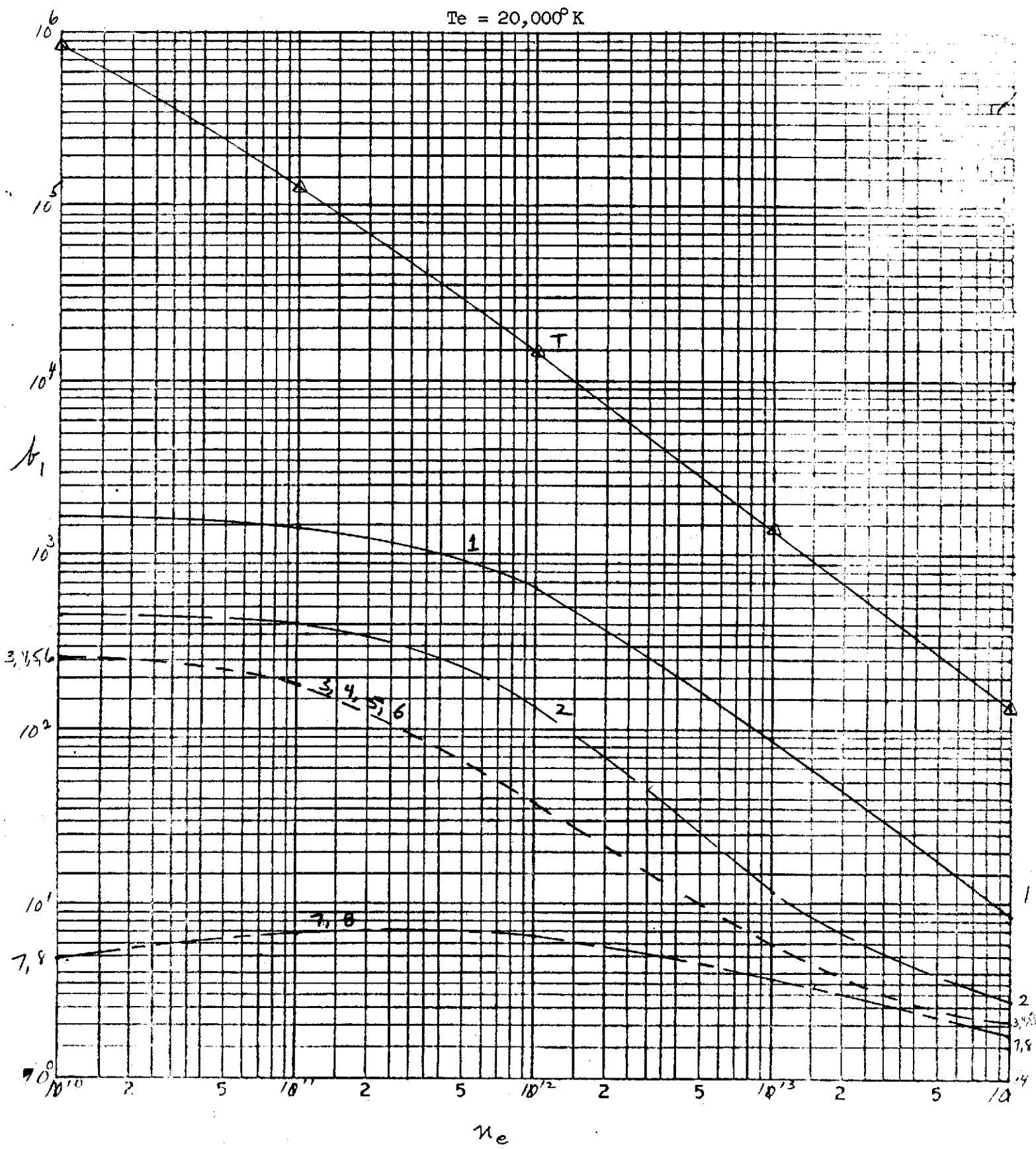
Figure II-10 b_1 

Figure II-11 b_5

$T_e = 20,000^\circ K$

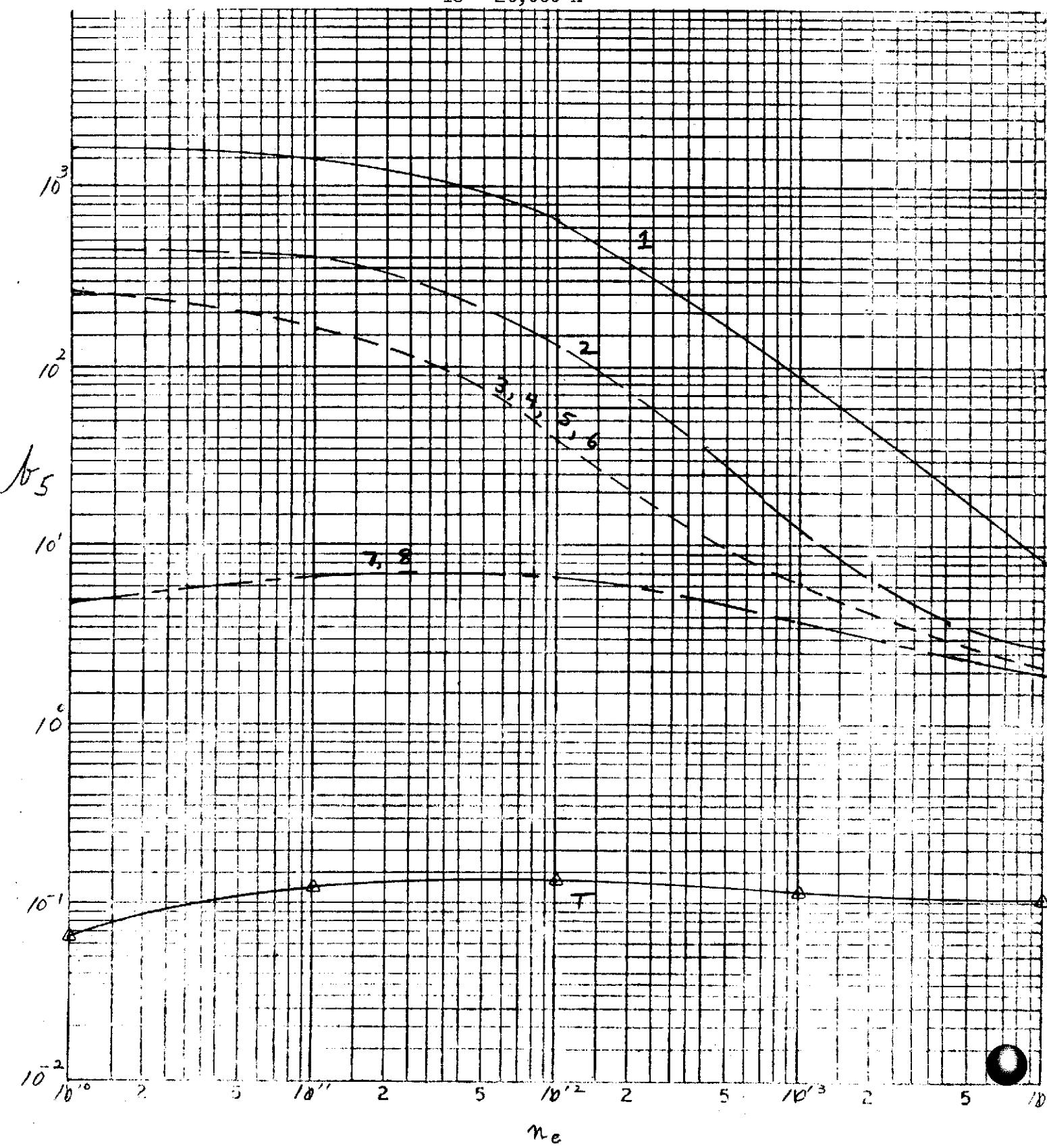


Figure II-12 b_9

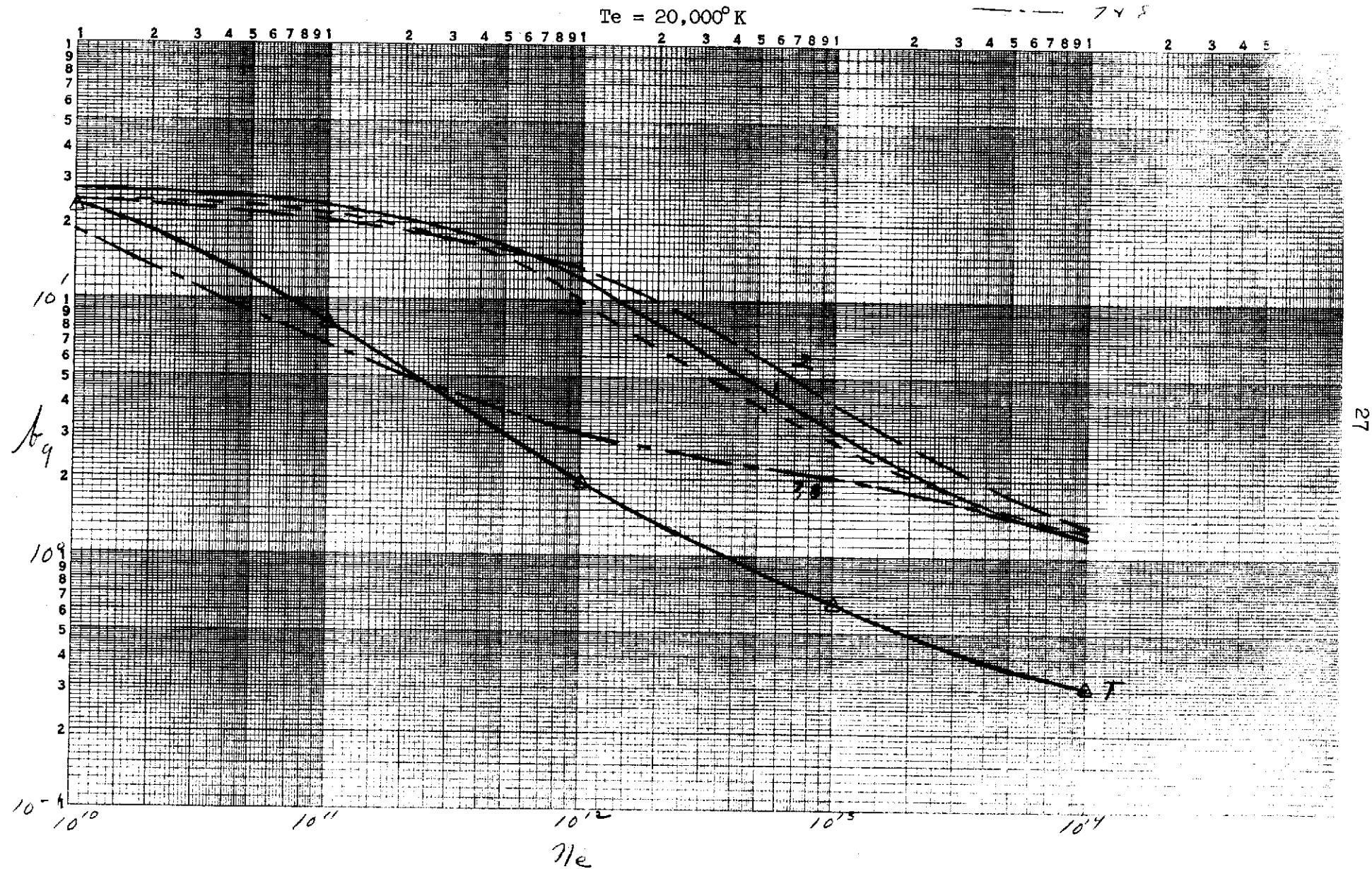


Figure II-13 b₂₇

T_e = 20,000° K

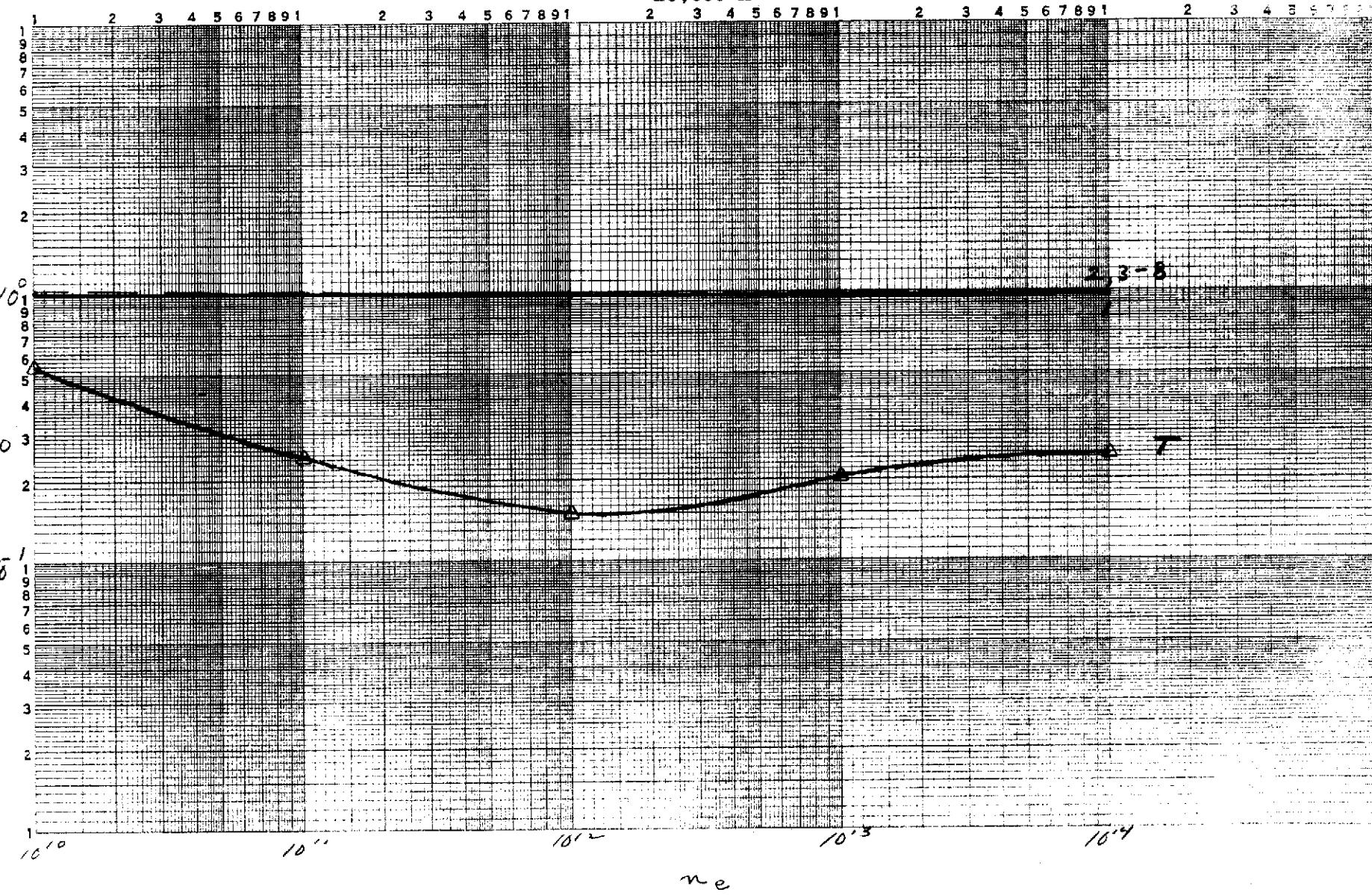


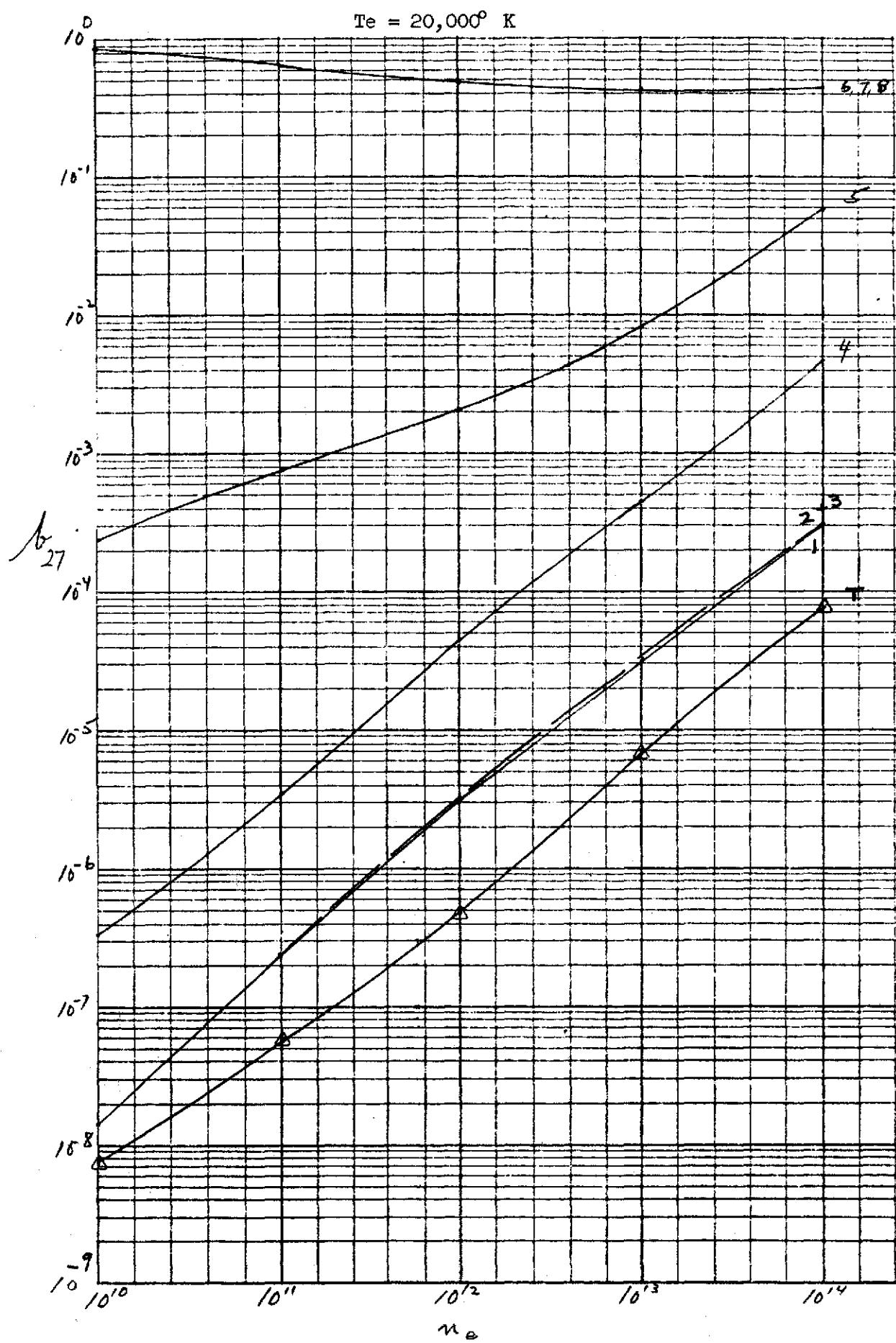
Figure II-14 b_{27} 

Figure II-15 b₅

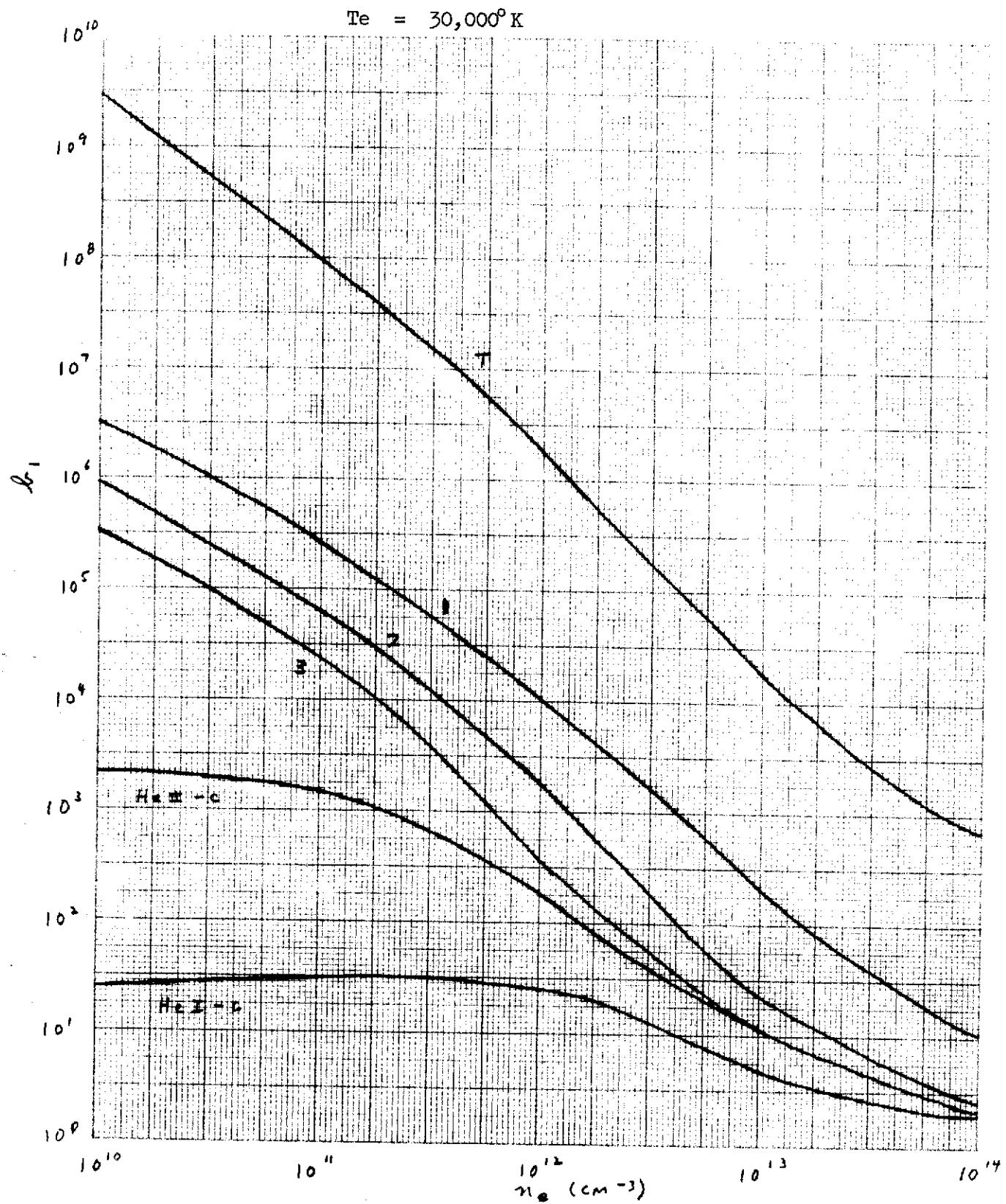


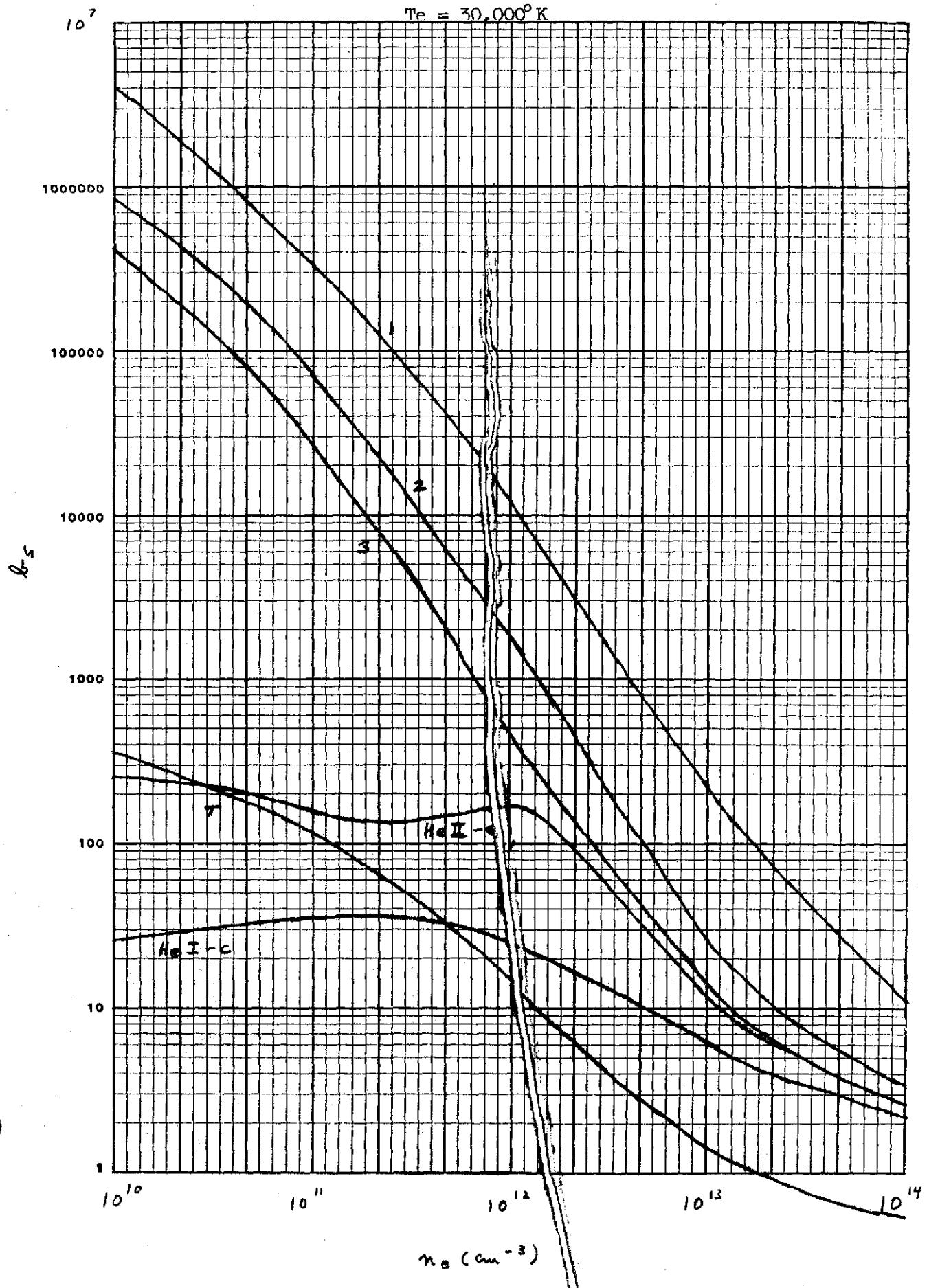
Figure II-16 b₅

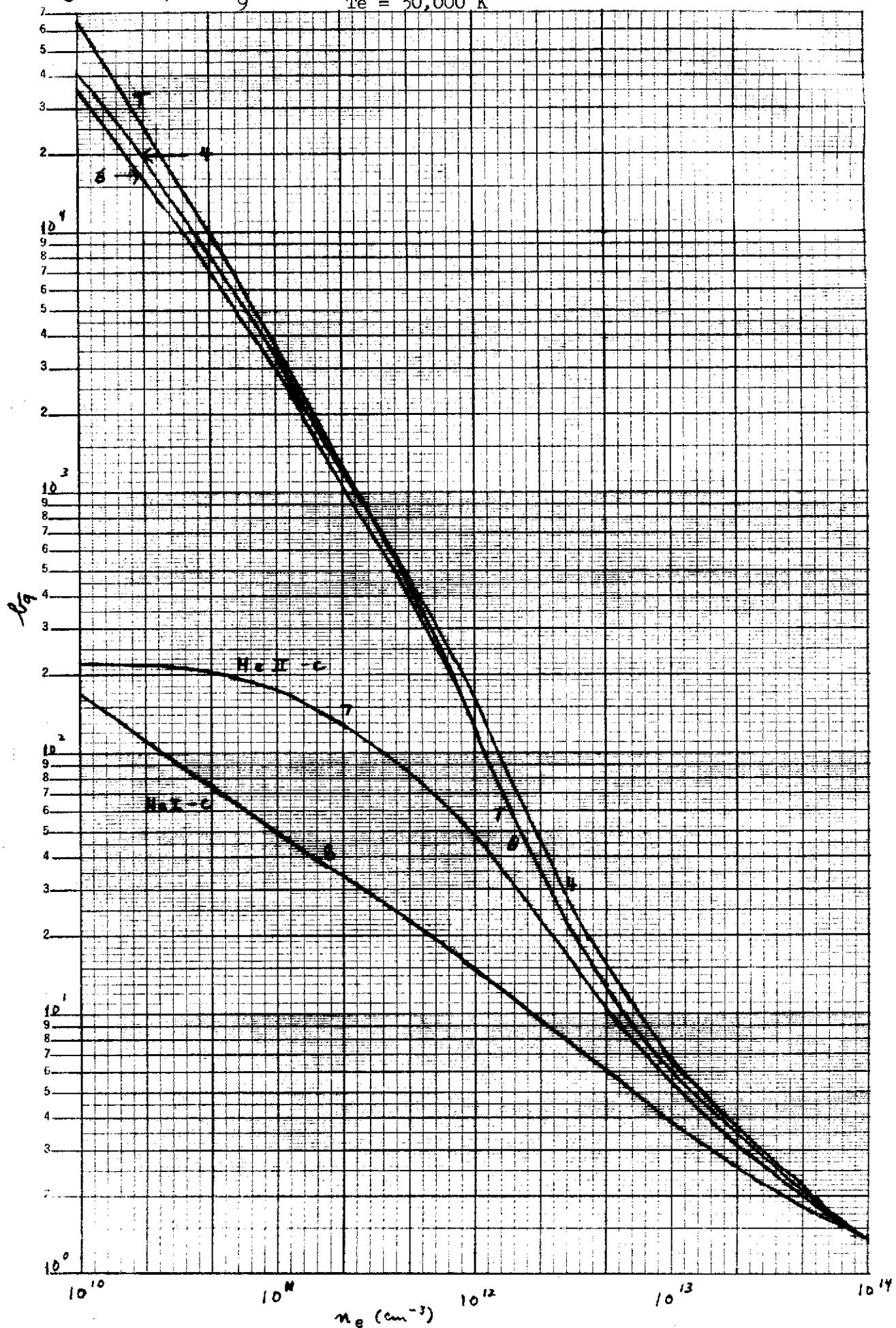
Figure II-17 b₉ $T_e = 30,000^\circ K$ 

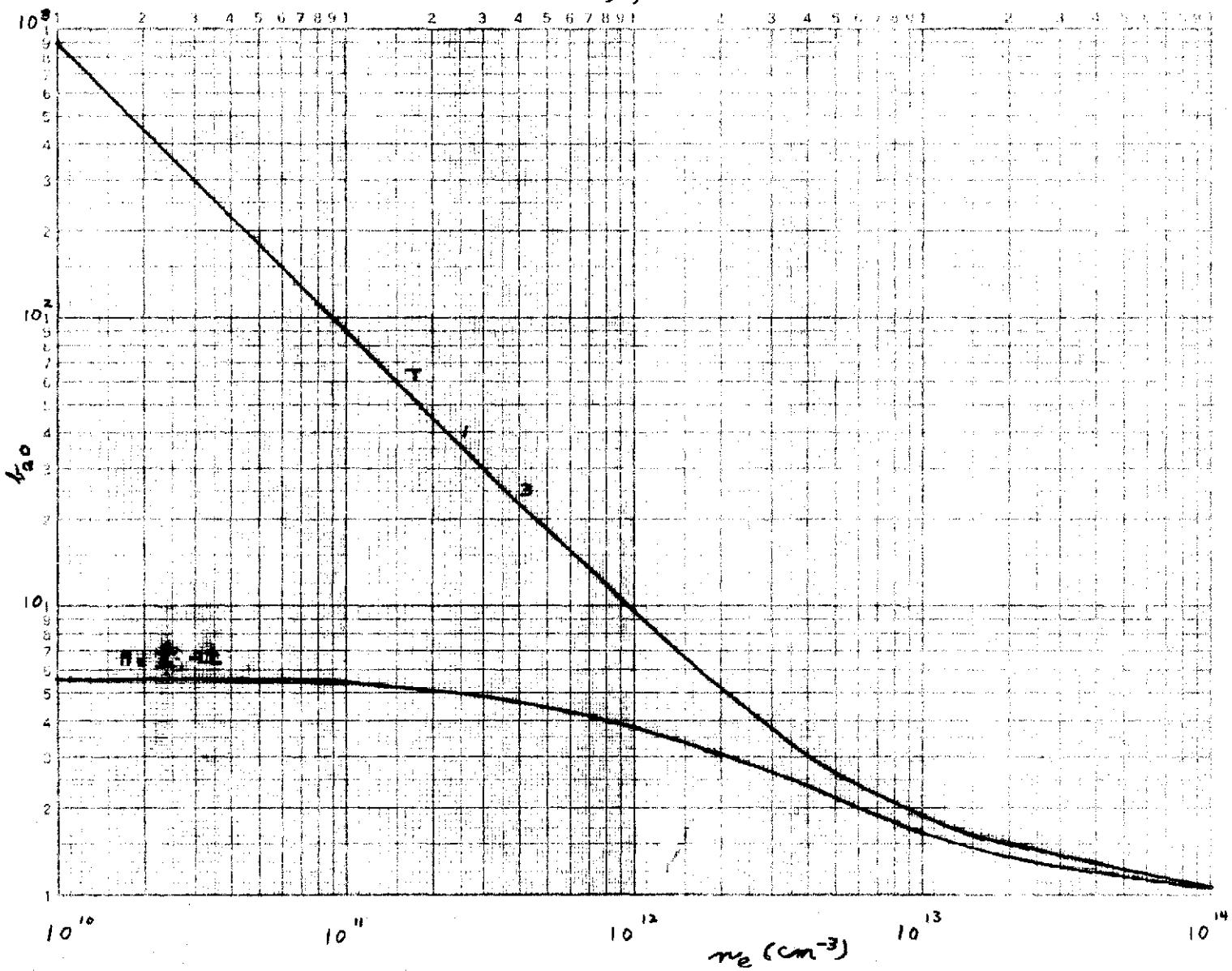
Figure II-18 b_{20} $T_e = 30,000^\circ K$ 

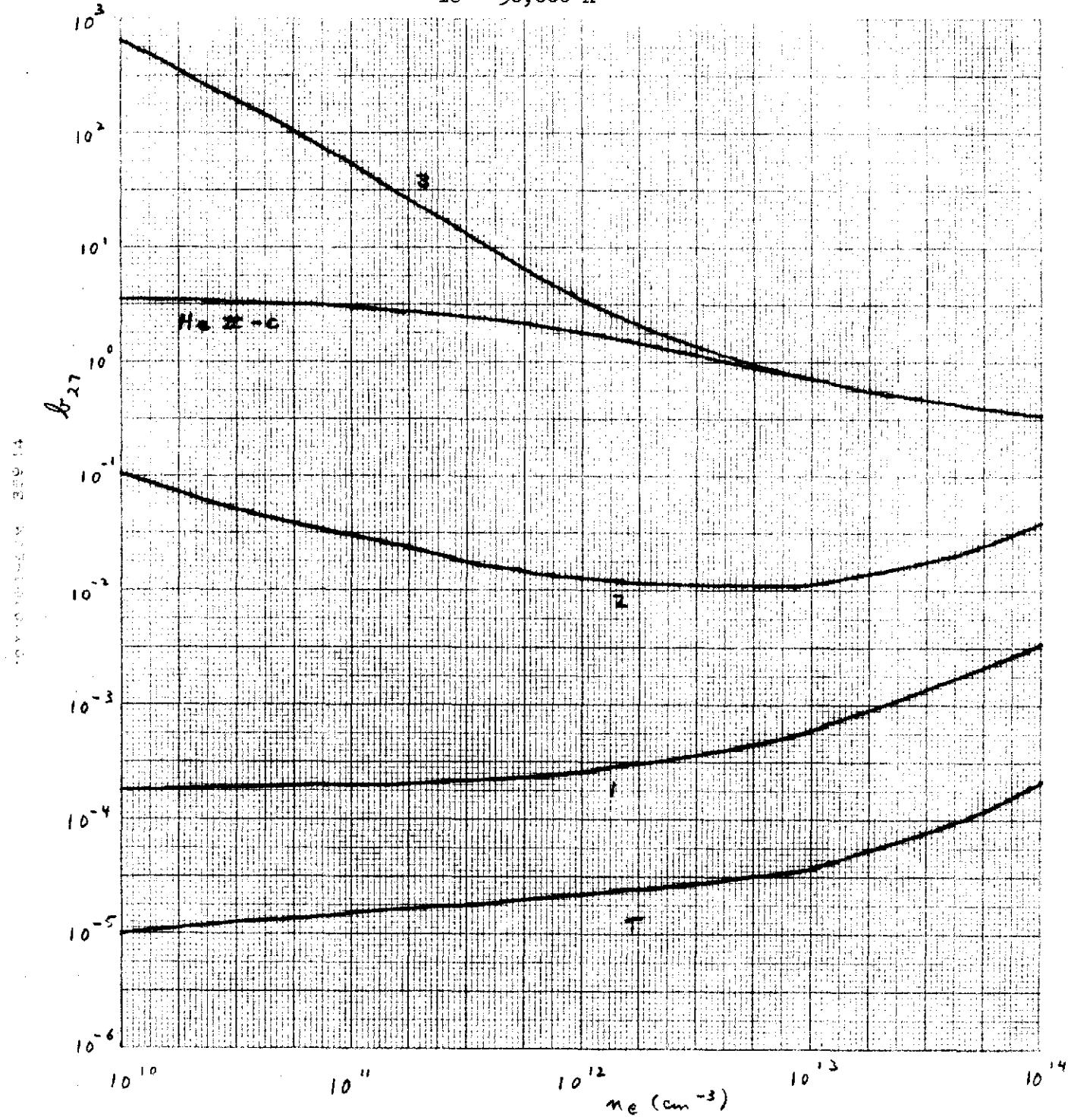
Figure II-19 b_{27} $T_e = 30,000^\circ K$ 

Figure II-20

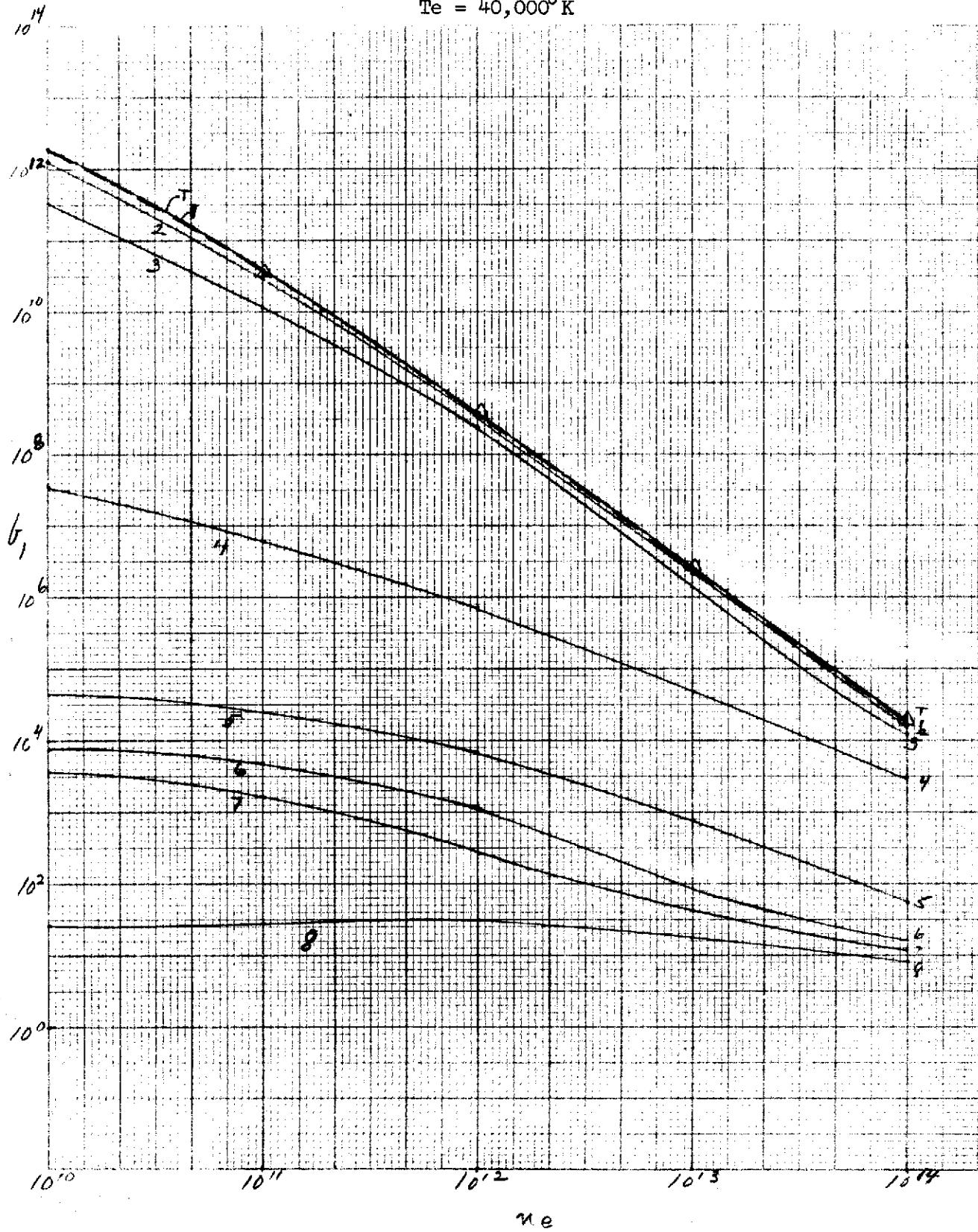
 b_1 $T_e = 40,000^\circ K$ 

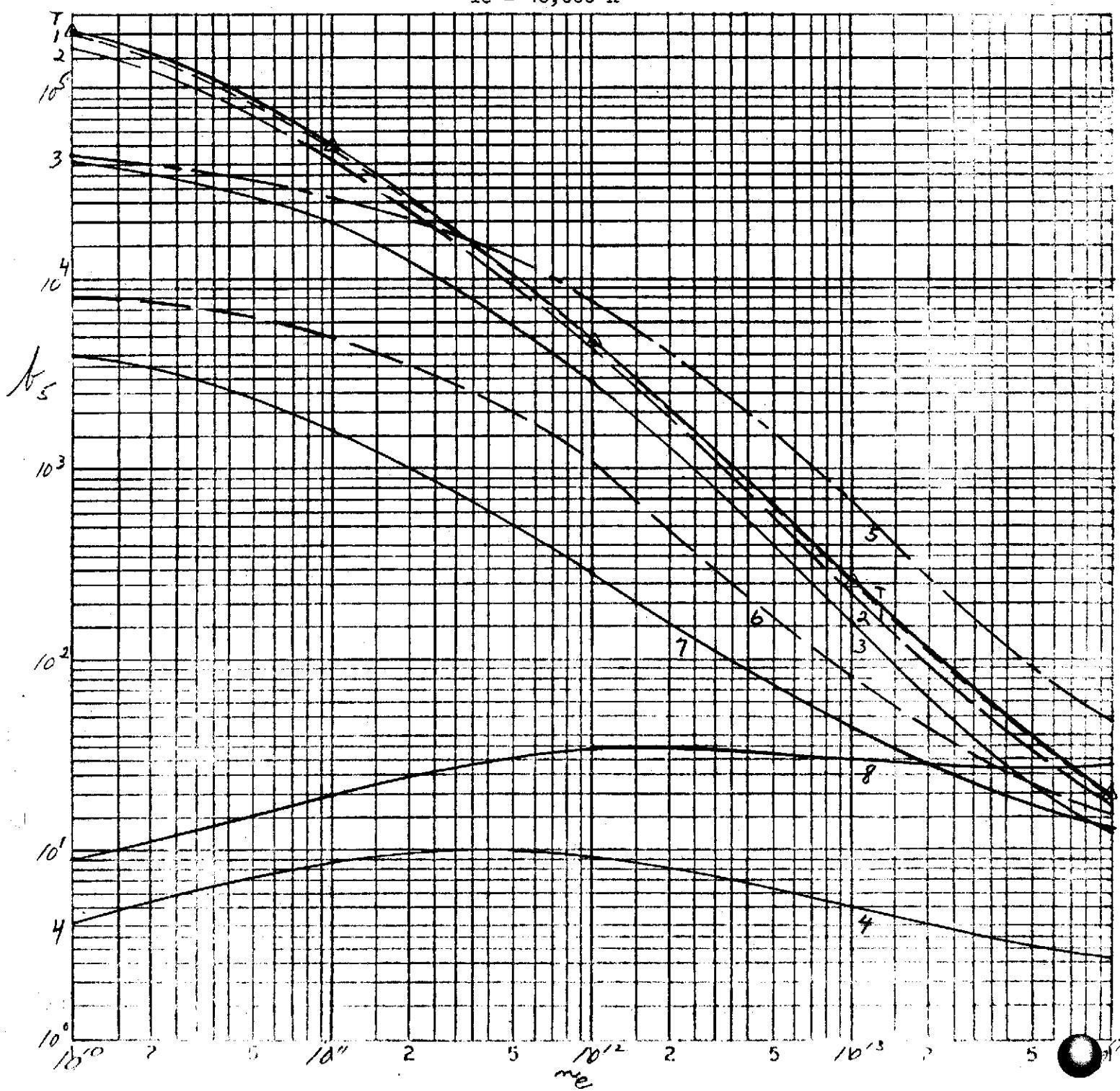
Figure II-21 b₅ $T_e = 40,000^{\circ}\text{K}$ 

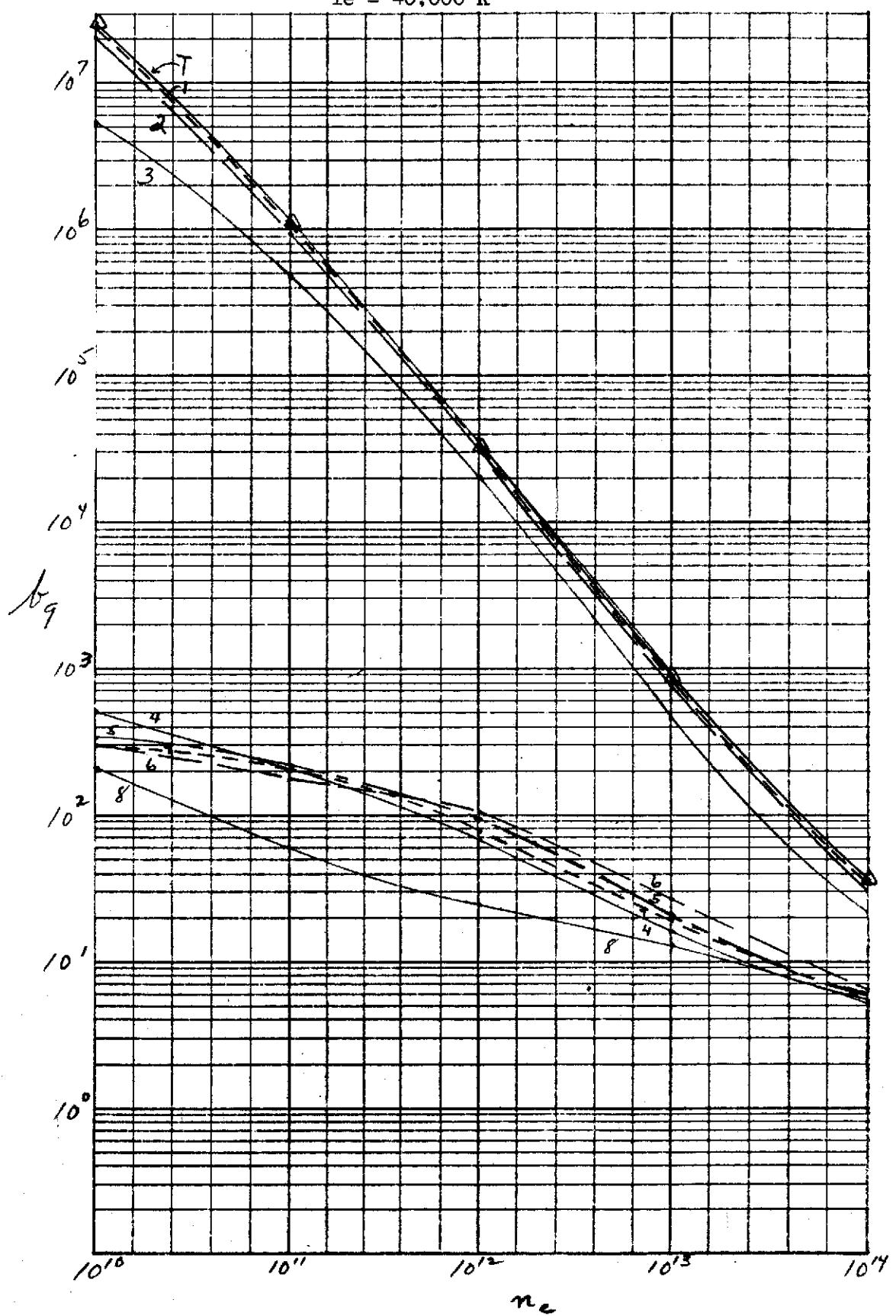
Figure II-22
b₉ $T_e = 40,000^\circ K$ 

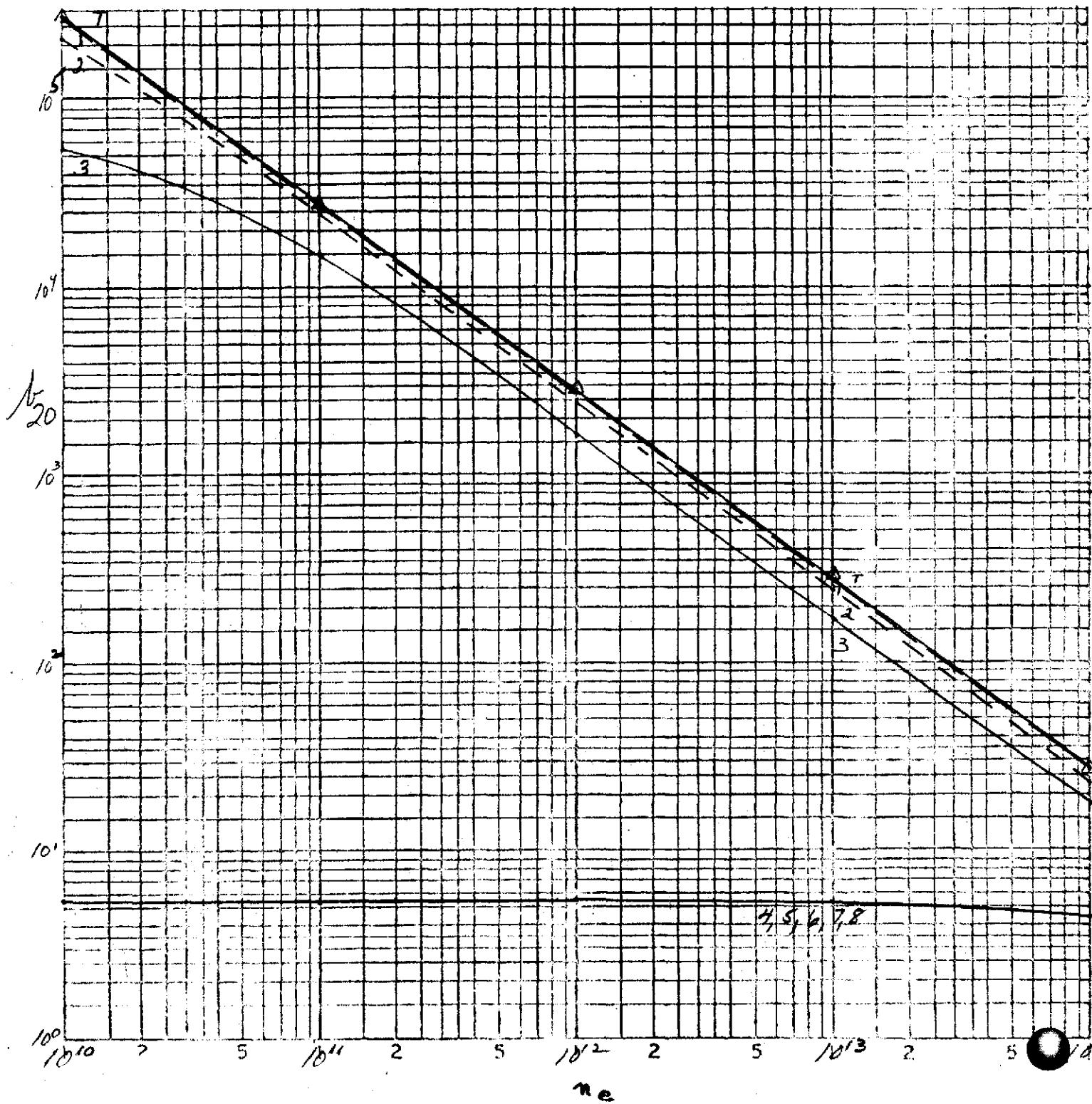
Figure II-23 b_{20} $T_e = 40,000^\circ K$ 

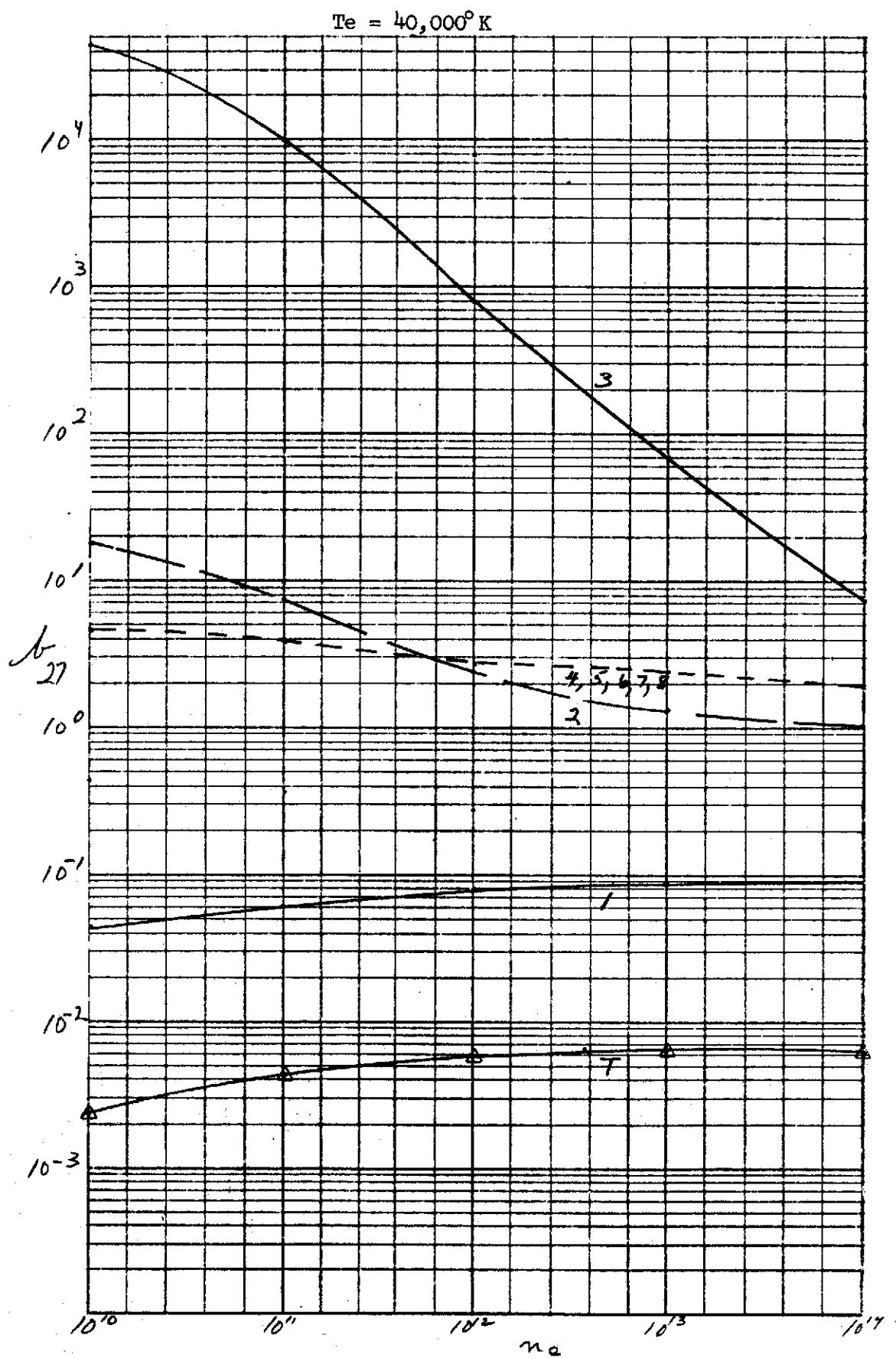
Figure II-24 b_{27} 

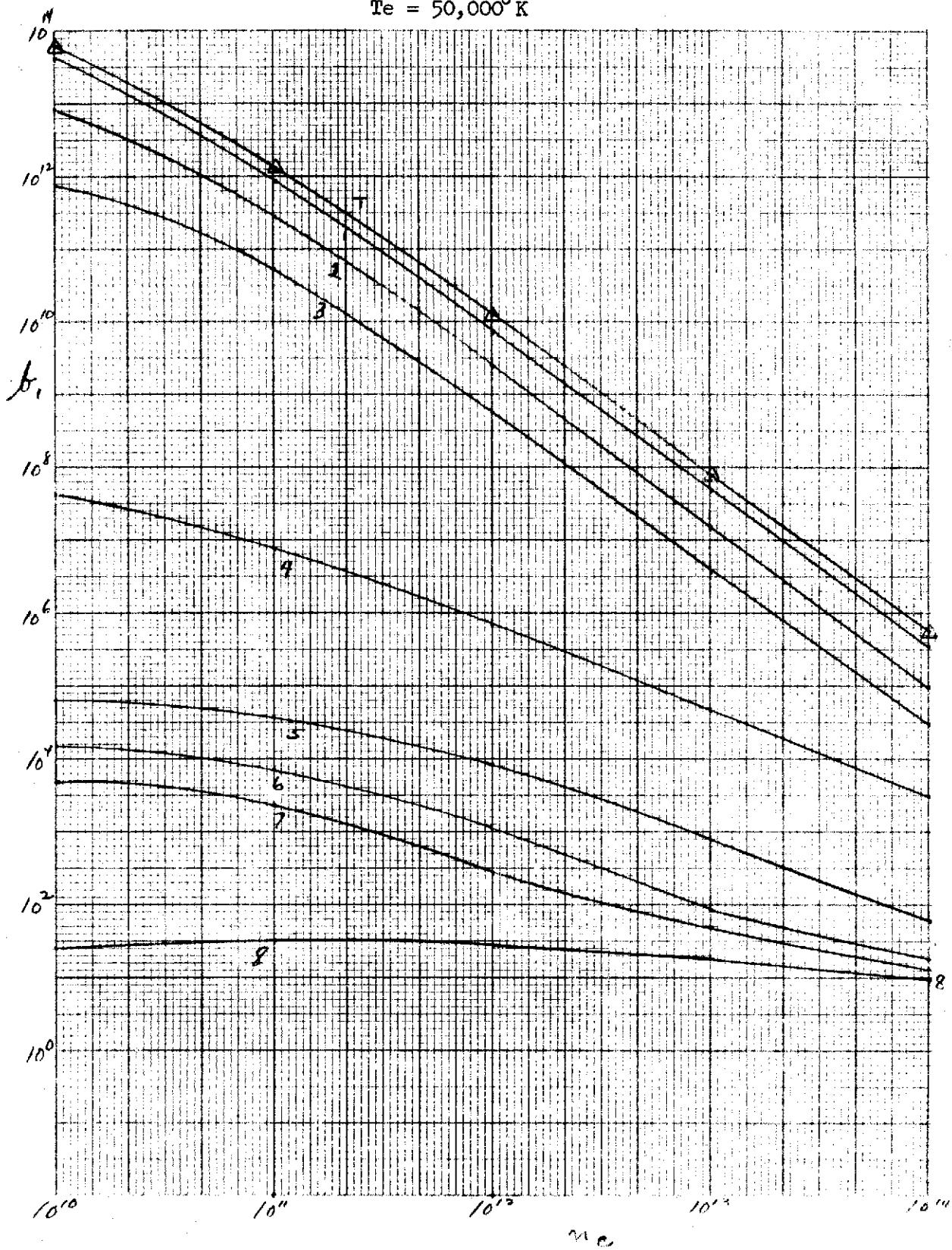
Figure II-25 b_1 $T_e = 50,000^\circ K$ 

Figure II-26

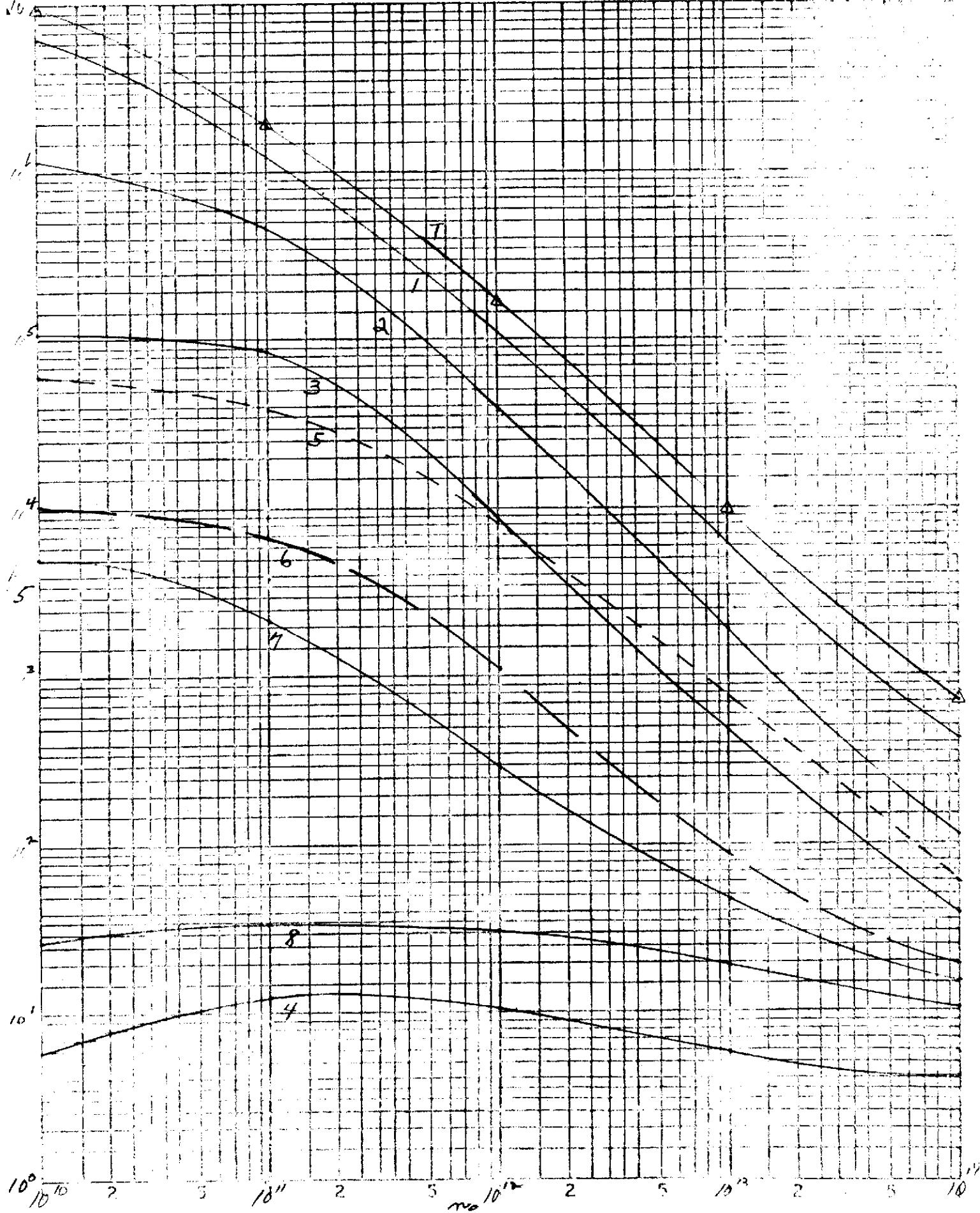
b
5 $T_e = 50,000^\circ K$ T_e

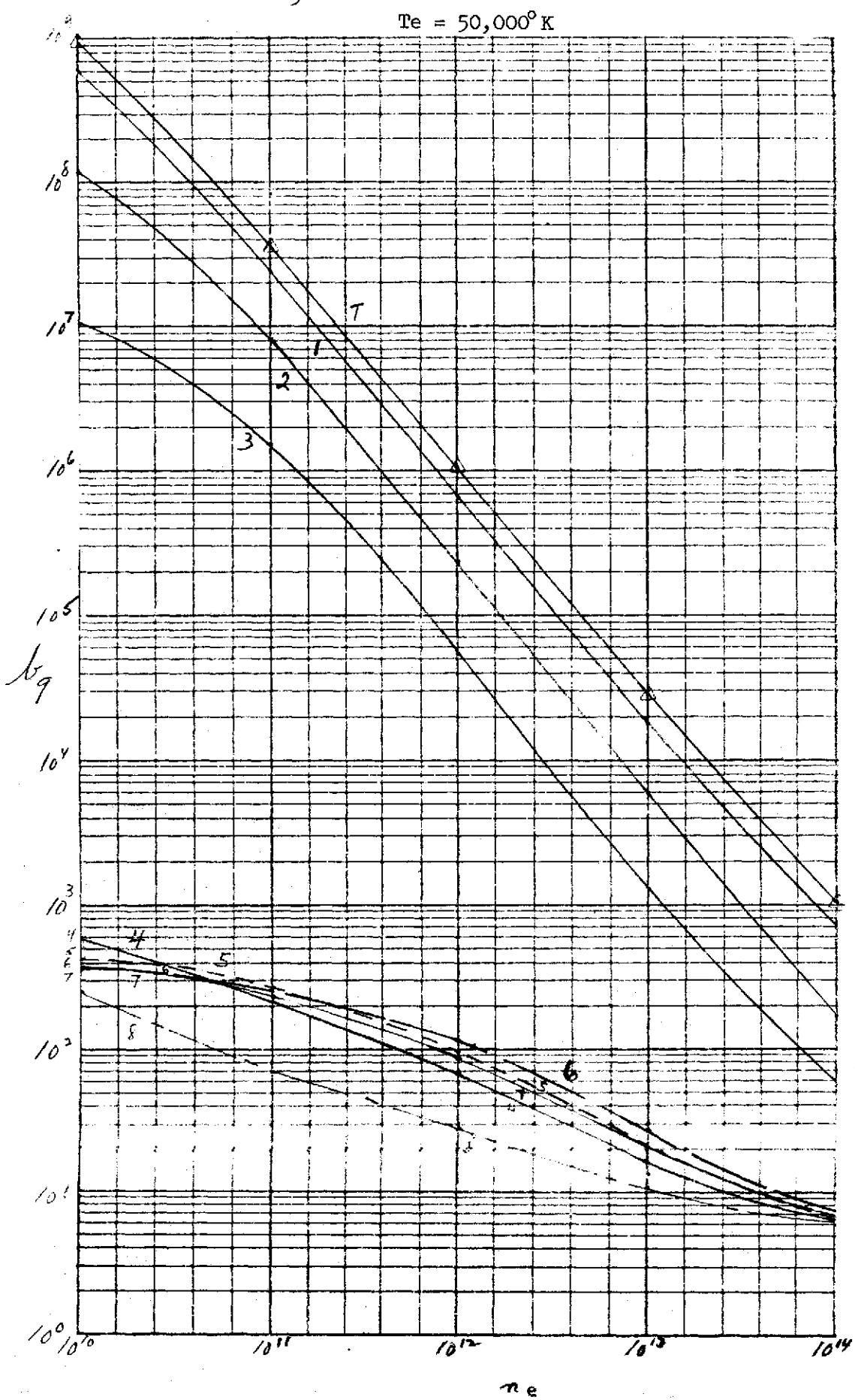
Figure III-27
 b_9 

Figure II-28

 b_{20}

43

$$T_e = 50,000^{\circ}K$$

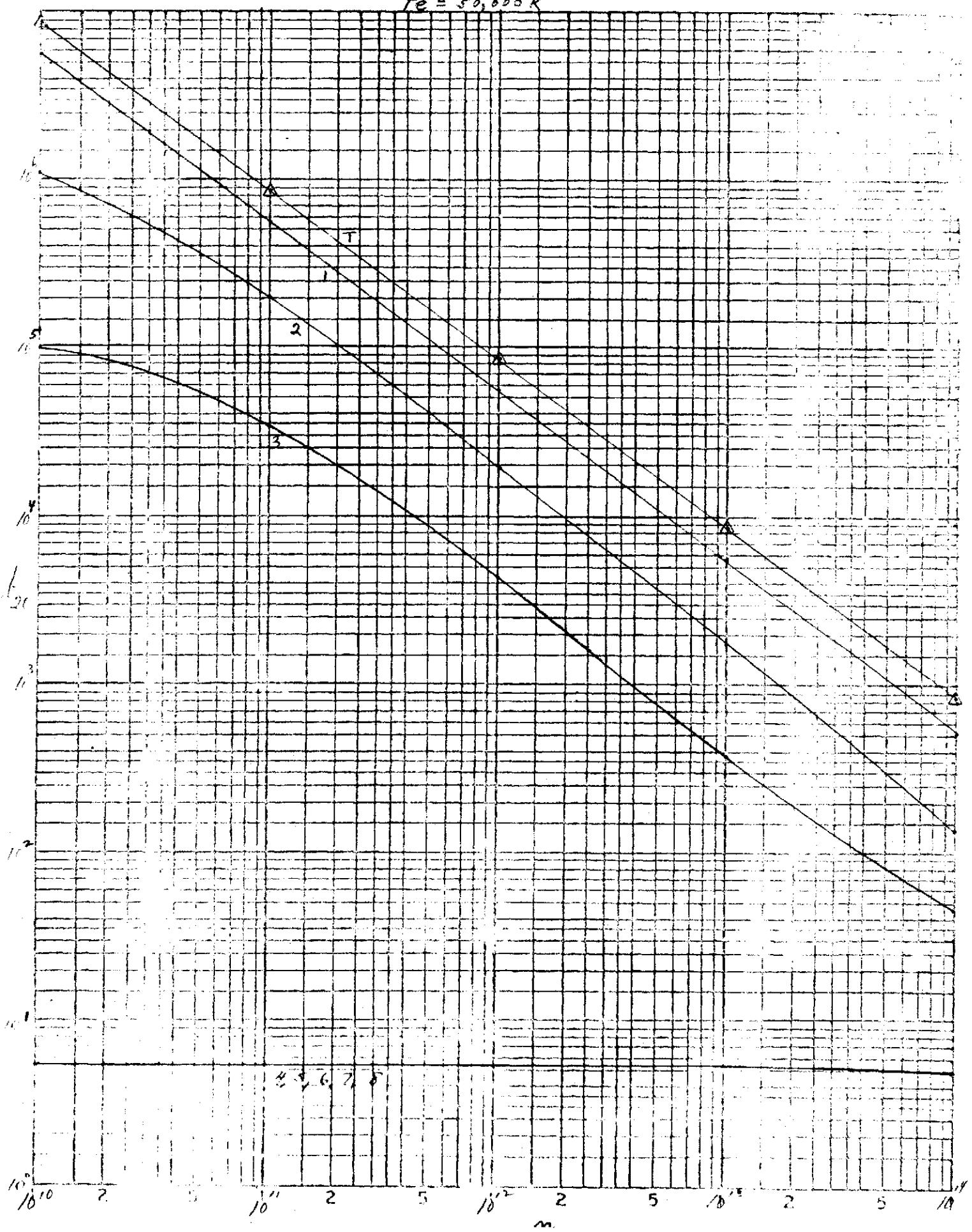
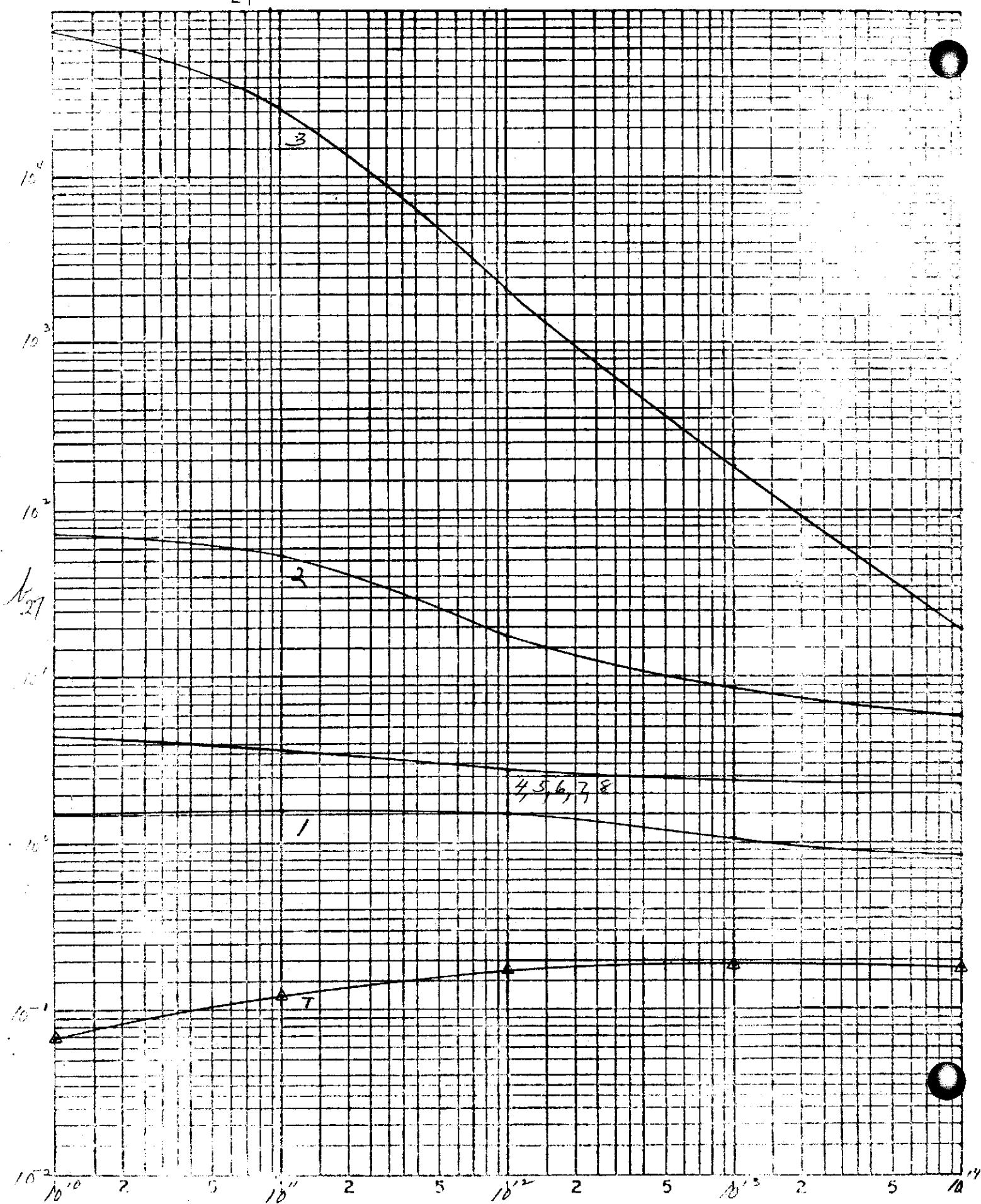


Figure II-29 b_{27} $T_e = 50,000^{\circ}K$ 

thicknesses given in Table II.3. On this table (1) refers to the 584 Å line, (2) refers to the 537 Å line, (3) refers to the 522 Å line and (4) refers to the Lyman continuum of He I. Similarly the numbers 5 - 8 refer to the 304, 256, 243 Å lines and Lyman continuum of He II. When a number appears in Table II.3 the corresponding transition has been assumed optically thick (i.e. in radiative detailed balance) in obtaining rate coefficients for the level population solutions. Transitions not appearing in the table are assumed optically thin. It is noted that progressing from case 1 to 8 corresponds in general to the layer becoming thicker. Case 8 always corresponds to all 8 lines and continua becoming optically thick. For example, with $T_e = 30,000^{\circ}\text{K}$ case 4 represents the NRB = 0 in the first 3 resonance lines of He I and the first resonance line of He II.

We shall discuss briefly the solutions presented in Figures II.5-30. For $T_e = 10^{40}^{\circ}\text{K}$ most of the He is He I. The He I ground state population is not affected by optical thickness except slightly at $n_e = 10^{10}$. Similarly Figure II.6 shows that once the 584 Å line becomes thick the radiation field in other lines and continua do not affect it. The D3 line upper level population shown in Figure II.7 is a strong function of the 584 Å line and He I Lyman continuum optical depths and to a lesser extent dependent on the 537 and 522 Å lines. Increasing the singlet populations hence increases the D3 emission. The optical thicknesses of the He II lines and continua do not affect the D3 line. From Figure II.8 it is seen that the He II ground state exhibits a similar behavior. At 20,000°K the He I and He II densities are very roughly the same. The thin solution shows that He I is greatly overpopulated and He II slightly underpopulated with respect to LTE. Increasing the optical depth in the He I resonance lines and continua now increases the ionization by absorption of photospheric radiation from upper resonance line levels and thus increases the He II density and decreases the He I density. The D3 line upper level population increases with increasing population of the singlet levels but decreases when the He I Lyman continuum becomes thick due to decreasing total He I density. As before the He II resonance line and continuum radiation fields do not affect the He I level populations.

At 30,000°K both He I and II ground states are overpopulated at the expense of He III. The He II ground state population is sensitive only to the Lyman continuum of He II while the He I population depends upon both continua and the

Table II-3
OPTICALLY THICK LINES CHOSEN

		Case Number							
		1	2	3	4	5	6	7	8
Temperature	10^4	1	1, 2	1-3	1-4	1-5	1-6	1-7	1-8
	2×10^4	1	1, 2	1-3	1-3	1-3	1-3	1-3	1-8
					5	5, 6	5-7	5-8	
	3×10^4	5	5, 6	5-7	1	1, 2	1-3	1-3	1-8
					5-7	5-7	5-7	5-8	
	4×10^4	5	5, 6	5-7	5-8	1	1, 2	1-3	1-8
						5-8	5-8	5-8	
	5×10^4	5	5, 6	5-7	5-8	1	1, 2	1-3	1-8
						5-8	5-8	5-8	

He I resonance lines. The D β line is sensitive only to the optical thickness in the two Lyman continua. The level 27 population depends upon the He II resonance lines and continua only. At $T_e = 40,000^\circ K$ all the levels have a strong dependence on the optical thickness of the He II Lyman continuum. When this continuum is thick the population of He III is greatly increased while those of He I and II are decreased, then decreasing all of the level populations. For levels 9 and 20 this continuum has the largest influence. Levels 1 and 5 are also dependent on the He I resonance line and continuum optical depths. At $50,000^\circ K$ the level populations have the same behavior as at $40,000^\circ K$.

3. Optical Thickness and Line Intensity

Figures II.5-29 have illustrated the effect of optical thickness in the resonance lines and continua on certain level populations. We now seek to determine the approximate optical depths of a flare layer. For purposes of illustration we consider a 1000 km thick layer. For each of the same cases given in Table II.3 we have obtained the line center optical thickness in the 584, 304, D3, 10830 Å lines and at the threshold of the Lyman continua of He I and II. Optical depths are not shown for the 537, 522, 256, 243 Å lines because they are always simply a constant fraction of the 584 and 304 Å line optical thicknesses, namely $\tau(537) = .27 \tau(584)$, $\tau(522) = .11 \tau(584)$, $\tau(256) = .19 \tau(304)$, and $\tau(243) = .070 \tau(304)$.

The optical thicknesses are given in Tables II.4 - II.8. The He density is assumed to be one tenth of the electron density. The number following each entry is the power of 10 by which the entry is multiplied. We note that the 10830 and D3 lines can become thick for high electron densities even at 50,000°K. These lines do not become thick at 10,000°K. There are many cases in which a number of lines and continua are optically thick. This does not mean however that simultaneous transport equations must be solved for these lines and continua. Which line and continuum radiation fields must be obtained simultaneously depends upon the level population being sought as well as the temperature, density and layer optical thickness. To determine the effect of various lines and continua on levels 1, 5, 9, 20 and 27 we can refer to Figures II.5 - 29. For example, Table II.9 shows the approximate maximum percentage error encountered in the D3 line upper level population by solving only for the lines and continua given in each box. The effect on any level can be obtained from the output from Code 1. Figures II.5 - 29 illustrate the effect of varying the NRB between 0 and 1. In practice when the layer becomes optically thick it does not usually become so thick that the NRB = 0. In order for the line radiation field to become saturated we require

$$\tau_o > (\epsilon + \eta)^{-1},$$

Table II-4

OPTICAL THICKNESS - 1000 KM LAYER

 $T_e = 10,000 \text{ } ^\circ\text{K}$

TRANSITION	n_e 10^{10}	T	Case							
			1	2	3	4	5	6	7	8
584		3.7+4	=	=	=	1.3+4	=	=	=	=
504		7.6	=	=	=	4.1	=	=	=	=
5876		2.8-8	1.1-5	2.1-5	2.7-5	8.0-4	=	=	=	=
10830		2.6-7	1.0-4	1.9-4	2.5-4	7.4-3	=	=	=	=
304		1.5-2	9.6			8.6+2	=	=	=	=
228		1.4-6	9.3-4	1.8-3	2.4-3	8.3-2	=	=	=	=
	10^{11}									
584		3.7+5	=	=	=	=	=	=	=	=
504		76	=	=	=	=	=	=	=	=
5876		1.3-6	1.7-4	2.2-4	3.7-4	6.7-3	=	=	=	=
10830		1.2-5	1.2-3	2.1-3	3.4-3	6.2-2	=	=	=	=
304		.046				1.6+3	=	=	=	=
228		4.4-6	1.0-3	1.9-3	3.1-3	.15	=	=	=	=
	10^{12}									
584		3.7+6	=	=	=	=	=	=	=	=
504		7.6+2	=	=	=	=	=	=	=	=
5876		1.5-5	1.1-3	2.4-3	4.7-3	1.5-2	=	=	=	=
10830		1.2-4	8.6-3	2.0-2	3.7-2	0.12	=	=	=	=
304		0.10				1.3+3	=	=	=	=
228		9.3-6	1.0-3	2.8-3	6.0-3	1.2-1	=	=	=	=
	10^{13}									
584		3.7+7	=	=	=	=	=	=	=	=
504		7.6+3	=	=	=	=	=	=	=	=
5876		2.1-4	1.0-2	3.1-2	4.1-2	6.2-2	=	=	=	=
10830		1.4-3	4.7-2	0.13	0.17	0.26	=	=	=	=
304		0.56		1.3+22	2.5+2	1.1+3	=	=	=	=
228		5.4-5	2.7-3	1.3-2	2.4-2	1.0-1	=	=	=	=
	10^{14}									
584		3.7+8	=	=	=	=	=	=	=	=
504		7.6+4	=	=	=	=	=	=	=	=
5876		5.6-3	0.15	0.24	0.26	0.29	=	=	=	=
10830		1.4-2	0.37	0.54	0.59	0.66	=	=	=	=
304		4.7	1.7+2	5.0+2	6.1+2	9.3+2	=	=	=	=
228		4.5-4	1.6-2	4.8-2	5.9-2	9.0-2	=	=	=	=

Table II-5

OPTICAL THICKNESS - 1000 KM LAYER

$$T_e = 2 \times 10^4 \text{ } ^\circ\text{K}$$

TRANSITION	n_e	T	Case							
			1	2	3	4	5	6	7	8
584	10^{10}	1.7+3	3.4	0.92	0.52	=	=	=	7.0-3	=
504		0.36	7.2-4	1.9-4	1.1-4	=	=	=	1.5-6	=
5876		1.7-3	1.8-3	1.7-3	=	=	=	=	9.6-4	=
10830		1.6-2	1.7-2	1.6-2	=	=	=	=	9.3-3	=
304		1.5+3	2.8+3	=	=	=	=	=	2.0+3	=
228		0.10	0.19	=	=	=	=	=	0.13	=
584	10^{11}	2.0+4	2.2+2	61.	26.	=	=	=	1.0	=
504		5.7	6.3-2	1.7-2	7.4-3	=	=	=	2.9-4	=
5876		4.3-2	0.11	=	=	=	=	=	3.3-2	=
10830		0.38	1.0	0.86	0.93	=	=	=	2.9-4	=
304		5.1+3	2.1+4	=	=	=	=	=	=	=
228		0.43	1.8	=	=	=	=	=	=	=
584	10^{12}	2.3+5	1.0+4	2.0+3	5.6+2	=	=	=	100.	=
504		65.	2.8	0.56	0.16	=	=	=	2.8-2	=
5876		0.90	4.3	4.0	3.1	=	=	=	1.0	=
10830		5.3	24.	22.	17.	=	=	=	=	=
304		3.3+4	2.0+5	=	=	=	=	=	=	=
228		2.7	16.	=	=	=	=	=	=	=
584	10^{13}	2.0+6	1.2+5	1.7+4	8.5+3	=	=	=	5.2+3	=
504		6.1+2	37.	5.2	2.6	=	=	=	1.6	=
5876		18.	63.	48.	38.	=	=	=	28.	=
10830		37.	1.3+2	90.	69.	=	=	=	52.	=
304		4.0+5	1.9+6	=	=	=	=	=	=	=
228		36.	170.	=	=	=	=	=	=	=
584	10^{14}	2.0+7	1.2+6	3.8+5	3.0+5	=	=	=	2.6+5	=
504		5.8+3	350.	110.	87.	=	=	=	75.	=
5876		2.8+2	7.7+3	5.4+2	5.1+2	=	=	=	4.8+2	=
10830		5.8+3	8.8+3	5.8+2	5.4+2	=	=	=	5.1+2	=
304		5.1+6	1.9+7	=	=	=	=	=	=	=
228		450.	1.7+3	=	=	=	=	=	=	=

Table II-6

OPTICAL THICKNESS - 1000 KM LAYER

$$T_e = 3 \times 10^4 \text{ K}$$

Table II-7

OPTICAL THICKNESS - 1000 KM LAYER

$$T_e = 4 \times 10^4 \text{ } ^\circ\text{K}$$

TRANSITION	n_e 10^{10}	T	Case							
			1	2	3	4	5	6	7	8
584	10^{10}	1.9	=	1.5	0.37	1.9-4	1.0-7	1.7-8	8.5-9	5.5-11
504		7.6-4	=	4.5-4	1.5-4	7.6-8	4.0-11	6.8-12	3.4-12	2.2-14
5876		8.3-4	=	6.4-4	1.6-4	1.6-8	1.4-8	1.2-8	=	6.6-9
10830		7.7-3	=	5.9-3	1.5-3	7.7-7	1.3-7	1.0-7	=	6.0-8
304		1.5+3	=	1.2+3	2.9+2	2.9-2	=	=	=	=
228		0.18	=	0.11	.035	3.5-6	=	=	=	=
584	10^{11}	40.	38.	33.	15.	6.7-3	4.3-5	8.0-6	2.7-7	4.7-9
504		1.7-2	=	1.5-2	7.0-3	2.8-6	1.8-8	3.4-9	1.1-10	2.0-12
5876		0.32	0.31	0.27	0.13	5.6-6	=	3.8-6	=	1.2-6
10830		0.26	0.25	0.21	0.11	4.5-5	=	3.9-5	=	1.3-5
304		1.4+4	=	1.3+4	7.6+3	2.8	=	=	=	=
228		1.8	=	1.6	0.81	3.6-4	=	=	=	=
584	10^{12}	4.2+2	4.1+2	3.7+2	2.5+2	0.82	8.1-3	1.1-3	2.5-4	3.3-5
504		0.17	=	0.15	0.11	3.4-4	3.4-6	4.7-7	1.2-7	1.4-8
5876		0.69	0.67	0.61	0.41	1.4-3	=	=	1.1-3	4.0-4
10830		2.6	2.5	2.3	1.5	5.0-3	=	4.9-3	4.0-3	1.4-3
304		1.5+5	1.4+5	1.3+5	8.7+4	2.9+2	=	=	=	=
228		18.	17.	16.	11.	3.6-2	=	=	=	=
584	10^{13}	2.7+3	2.5+3	2.3+3	1.6+3		0.80	0.10	4.5-2	2.0-2
504		1.0	0.92	0.84	0.68	2.2-2	2.1-4	3.6-5	1.8-5	7.7-6
5876		9.1	8.7	8.0	5.6	0.19	0.16	0.13	0.10	8.0-2
10830		11.	10.	9.2	6.5	0.22	0.19	0.14	0.12	8.5-2
304		1.5+6	1.4+6	1.2+6	8.8+5	3.0+4	=	=	=	=
228		180.	170.	160.	100.	3.6	=	=	=	=
584	10^{14}	2.1+4	2.0+4	1.7+4	1.2+4	3.1+3				9.0
504		8.4	7.8	6.4	3.0	0.77	1.3-2	4.0-3	3.2-3	2.2-3
5876		99.	95.	83.	58.	15.	12.	10.	9.0	8.3
10830		76.	72.	62.	45.	11.	10.	7.0	6.6	6.0
304		1.4+7	=	1.2+7	9.0+6	2.3+6	=	=	=	=
228		1.8+3	1.7+3	1.4+3	1.2+3	3.0+2	=	=	=	=

Table II-8
OPTICAL THICKNESS - 1000 KM LAYER
 $T_e = 5 \times 10^4$ °K

TRANSITION	n_e 10^{10}	T	Case							
			1	2	3	4	5	6	7	8
584		0.35	0.21	4.2-2	3.5-3	2.1-7	-	-	-	-
504		1.5-4	9.0-5	1.8-5	1.5-6	9.0-11	-	-	-	-
5876		5.4-4	3.4-4	6.5-5	5.3-6	3.2-10	-	-	-	-
10830		4.9-3	3.0-3	6.0-4	5.0-5	3.0-9	-	-	-	-
304		1.3+3	7.8+2	1.6+2	13.	7.8-4	=	=	=	=
228		0.18	0.11	2.2-2	1.8-3	1.1-7	=	=	=	=
	10^{11}									
584		6.6	4.0	1.3	0.26	4.0-5	-	-	-	-
504		3.0-3	1.8-3	5.9-4	1.2-4	1.8-8	-	-	-	-
5876		1.8-2	1.1-2	3.6-3	7.2-4	1.1-7	-	-	-	-
10830		0.14	8.4-2	2.8-2	5.6-3	8.4-7	-	-	-	-
304		1.3+4	7.8+3	2.6+3	5.2+2	7.8-2	=	=	=	=
228		1.8	1.1	0.36	7.2-2	1.1-5	=	=	=	=
	10^{12}									
584		62.	37.	12.	3.1	3.7-3	-	-	-	-
504		3.0-2	1.8-2	5.8-3	1.5-3	1.8-6	-	-	-	-
5876		0.37	0.22	7.4-2	1.8-2	2.2-5	-	-	-	-
10830		1.2	0.75	0.24	6.0-2	7.2-5	-	-	-	-
304		1.3+5	7.8+4	2.6+4	6.5+3	7.8	=	=	=	=
228		18.	11.	3.6	0.90	1.1-3	=	=	=	=
	10^{13}									
584		4.1+2	2.4+2	82.	20.	0.25	4.0-3	4.5-4	2.3-4	9.0-5
504		0.18	0.11	3.6-2	8.8-3	1.1-4	1.8-6	2.0-7	1.0-7	4.0-8
5876		4.8	2.9	0.96	0.24	2.9-3	2.6-3	2.2-3	1.7-3	1.3-3
10830		4.9	2.9	1.0	0.25	2.9-3	2.6-3	2.1-3	1.7-3	1.3-3
304		1.3+6	7.8+5	2.6+5	6.5+4	7.8+2	=	=	=	=
228		180.	110.	36.	8.8	0.11	=	=	=	=
	10^{14}									
584		3.0+3	1.9+3	5.0+2	160.	19.	0.35	0.11	8.5-2	5.9-2
504		1.4	0.84	0.22	7.0-2	8.9-3	1.6-4	5.1-5	4.0-5	2.8-5
5876		47.	30.	7.8	2.4	0.29	0.25	0.20	=	=
10830		33.	21.	5.6	1.7	0.21	0.18	0.14	=	=
304		1.3+7	7.8+6	2.1+6	6.5+5	7.8+4	=	=	=	=
228		1.3+3	1.1+3	2.9+2	9.0+1	11.	=	=	=	=

Table III-9 ERROR IN D3 Line Intensity

He I - D3 LINE

	1, 2, 4	1, 2, 4	1, 2, 4	1, 2	1, 2
10^4 K	1, 2, 4 20%	1, 2, 4 40%	1, 2, 4 50%	1, 2 40%	1, 2 25%
$2 \times 10^4 \text{ K}$	T 20%	1, 4 5%	1, 4 20%	1, 4 25%	1 10%
$3 \times 10^4 \text{ K}$	1, 4, 8 10%	4, 8 5%	4, 8 1%	4 30%	T 1%
$4 \times 10^4 \text{ K}$	4, 7, 8 40%	4, 7, 8 5%	4, 7, 8 10%	4, 7, 8 10%	4, 7 10%
$5 \times 10^4 \text{ K}$	4, 5, 6, 7, 8 50%	4, 5, 6, 7, 8 10%	4, 5, 6, 7, 8 15%	4, 5, 6, 7, 8 10%	4, 5, 6, 7 5%
	10^{10}	10^{11}	10^{12}	10^{13}	10^{14}

 $n_e (\text{cm}^{-3})$

NUMBER RES. LINE	1 1 st	2 2 nd	3 3 rd	4 Ly- α	5 1 st	6 2 nd	7 3 rd	8 Ly- α
He I	He I	He I	He I	He I	He II	He II	He II	He II

TABLE II.10
CHARACTERISTIC VALUES OF ϵ , η , ζ

T_e ($^{\circ}$ K)	n_e (cm^{-3})	ϵ	η	ζ	Line (\AA)	Case #
10^4	10^{10}	4.1-9	2.3-4	2.9-18	584	T
		"	"	5.1-14	"	3
		1.2-8	1.2-8	1.8-28	304	T
		"	"	"	"	3
	10^{14}	4.0-5	8.0-3	4.0-14	584	T
		"	"	8.3-13	"	3
		1.2-4	4.8-5	1.8-24	304	T
		"	"	"	"	3
2×10^4	10^{10}	1.1-8	2.3-4	6.1-13	584	T
		"	"	3.8-3	"	3
		8.2-9	1.2-8	2.5-18	304	T
		"	"	"	"	3
	10^{14}	1.1-4	2.2-2	6.4-9	584	T
		"	"	4.9-7	"	3
		8.2-5	5.8-5	2.5-14	304	T
		"	"	"	"	3
3×10^4	10^{10}	1.9-8	2.3-4	4.3-11	584	T
		"	"	"	"	3
		6.7-9	1.4-8	6.1-15	304	T
		"	"	4.2-9	"	3
	10^{14}	6.7-5	1.2-4	5.8-11	584	T
		"	"	1.4-8	"	3
		1.9-4	3.4-2	4.0-7	304	T
		"	"	"	"	3
4×10^4	10^{10}	2.8-8	2.3-4	3.9-10	584	T
		"	2.1-4	2.9-10	"	3
	10^{14}	5.8-9	1.6-8	3.1-13	304	T
		"	"	4.7-7	"	3

TABLE II.10(Continued)

$T_e(^{\circ}\text{K})$	n_e (cm^{-3})	ϵ	η	ℓ	Line (\AA)	Case #
5×10^4	10^{14}	2.8-4	4.5-2	3.4-6	584	T
		"	"	"	"	3
	10^{10}	5.8-5	1.9-4	2.8-9	304	T
		"	"	1.9-6	"	3
	10^{14}	3.8-8	2.3-4	1.6-9	584	T
		"	2.0-4	9.0-10	"	3
		5.2-9	1.9-8	3.4-12	304	T
		"	"	8.1-6	"	3
	10^{14}	3.8-4	2.7-4	3.0-8	304	T
		"	5.8-2	"	"	3
		5.2-5	2.7-4	3.0-8	304	T
		"	"	2.7-5	"	3

for our assumed Doppler line profile. (For the continuum we require $\tau > \zeta^{-1/2}$ where ζ is the ratio of collisional to radiative recombination.)

Some representative values of the parameters ϵ and η (and ζ) for the 584 and 304Å lines are given in Table II.10. Values were obtained for each temperature at $n_e = 10^{10}$ and 10^{14} for the optically thin case and case 3 given in Table II.3. We can see from the optical depth tables that under many conditions the layer is effectively optically thin, i.e.

$$1 < \tau \leq (\epsilon + \eta)^{-1}$$

In this case the total energy emitted in the line from the surface of a layer of optical thickness t_1 is given approximately by

$$E \sim 2\sqrt{\pi} (\epsilon + \eta^*) t_1$$

where $\eta^* = L/B$.

The values of η and ζ vary with optical depth and an integration over depth is required to obtain the total line intensity from the layer.

Using the optical depth tables and estimates of η and ζ from code 1 we have obtained approximate solutions for some line intensities. The lines chosen are the 584, 537, 304Å lines and the D3 line. Figures II.30-34 give results as a function of T_e for various n_e while Figures II.35-39 show the variation with n_e for various T_e . We note a considerably different variation with T_e and n_e for the D3, 584 and 304Å line emission. These different variations give some confidence that simultaneous emission measurements of the three lines could yield unique temperatures and densities from the emitting region.

Figure II-30 TOTAL LINE EMISSION

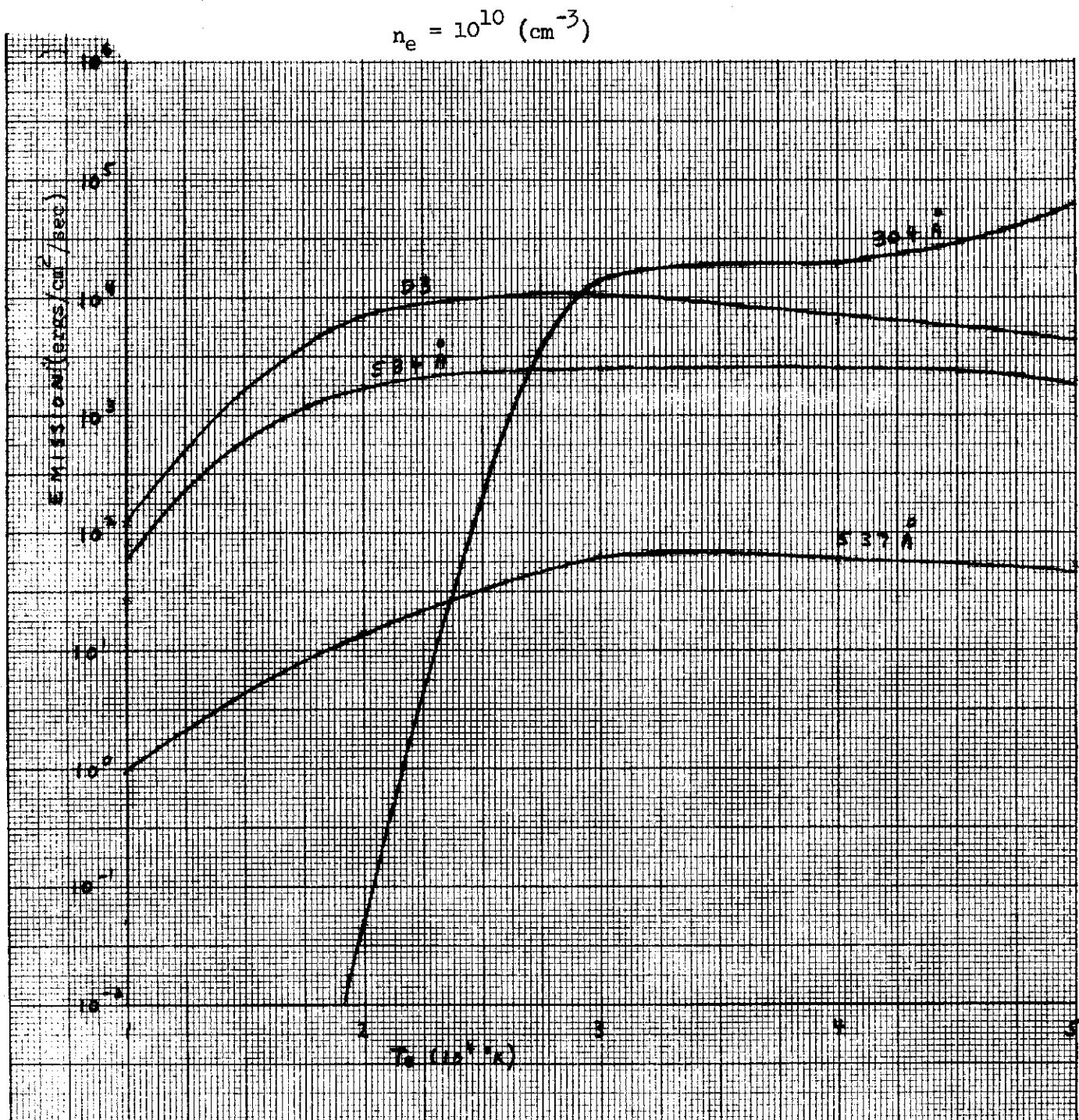


Figure II-31 TOTAL LINE INTENSITY

$$n_e = 10^{11} (\text{cm}^{-3})$$

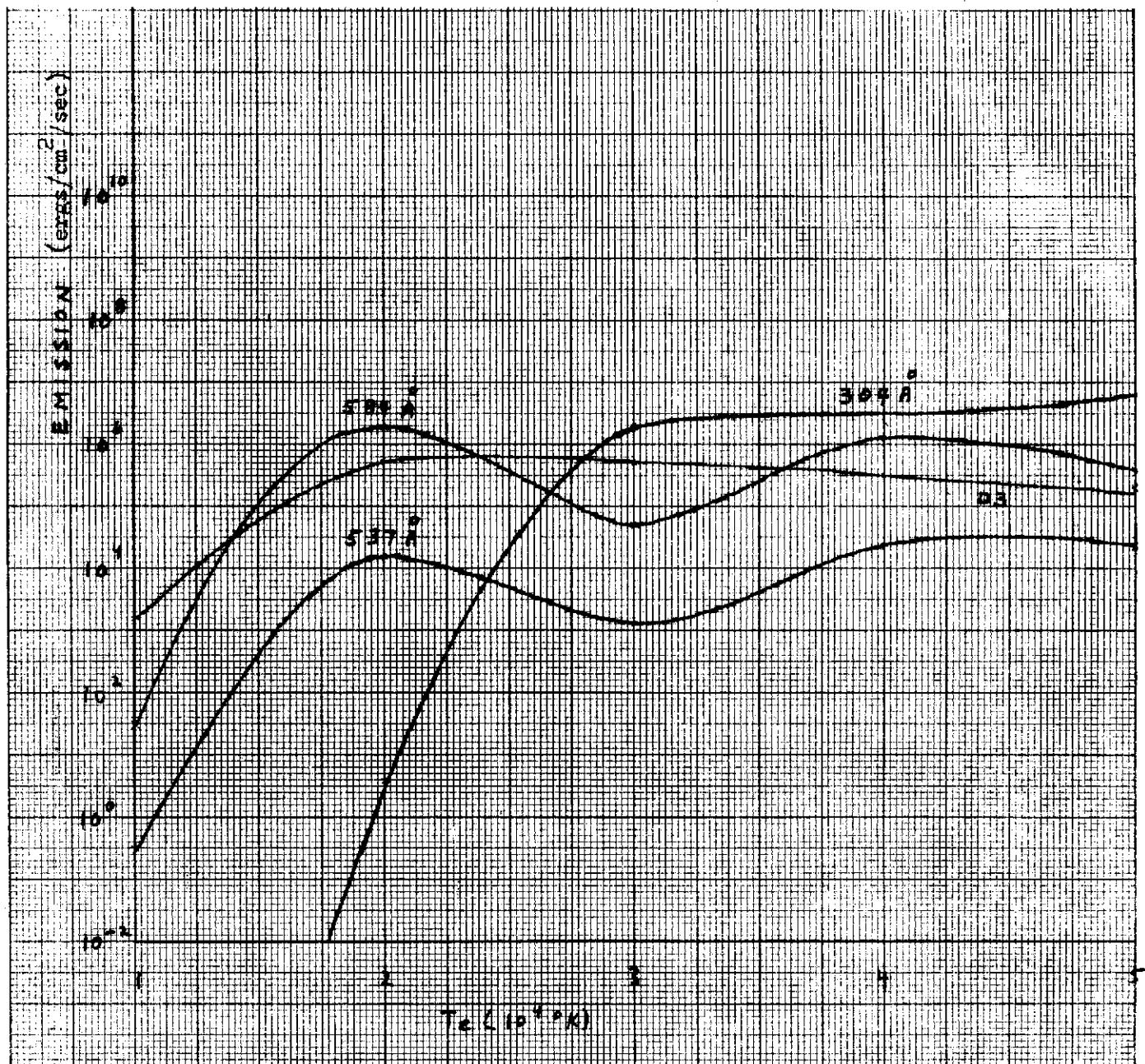


Figure II-32 TOTAL LINE EMISSION

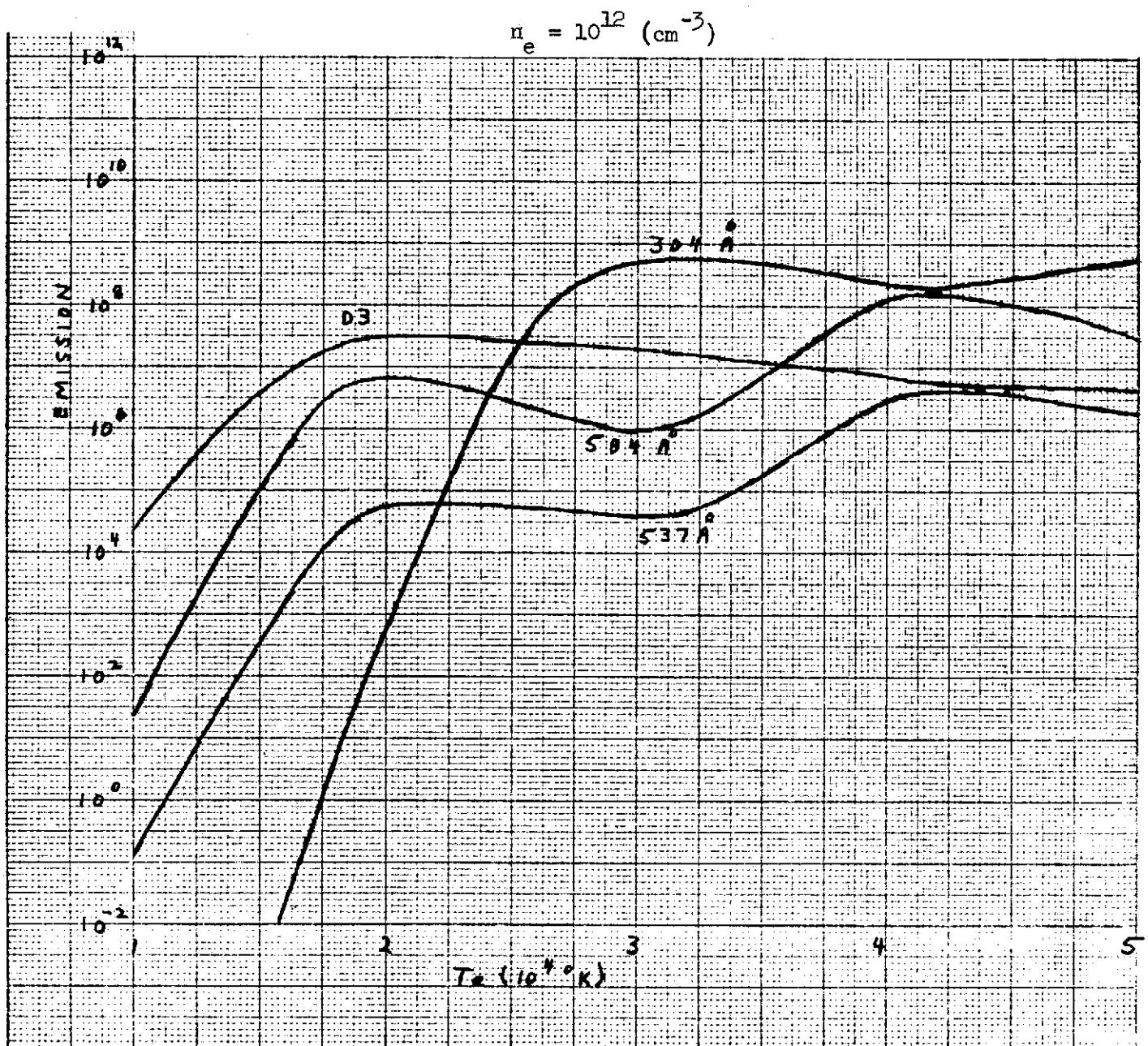


Figure II-33 TOTAL LINE EMISSION

$$n_e = 10^{13} \text{ (cm}^{-3}\text{)}$$

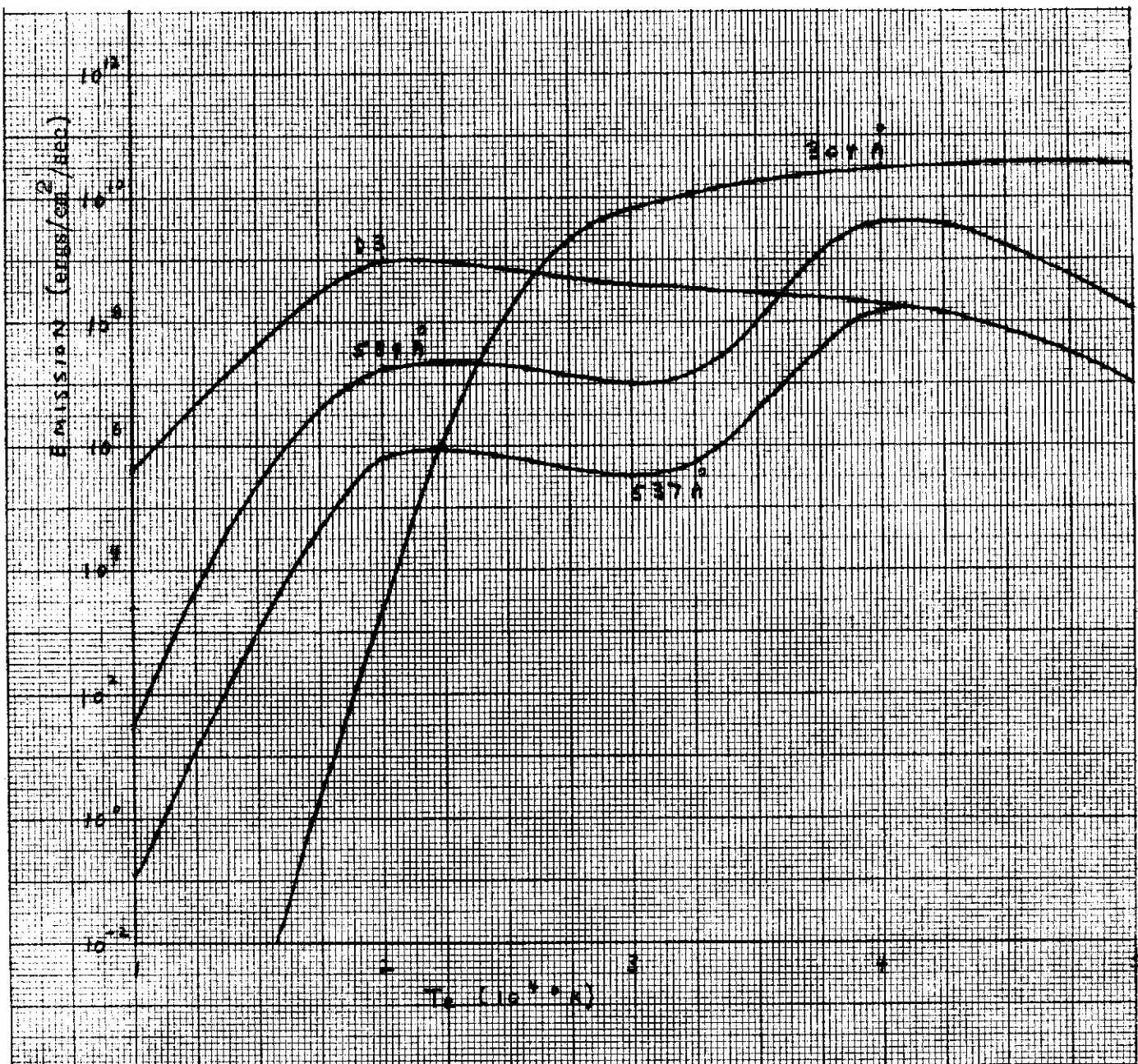


Figure II-34 TOTAL LINE EMISSION

$$n_e = 10^{14} \text{ (cm}^{-3}\text{)}$$

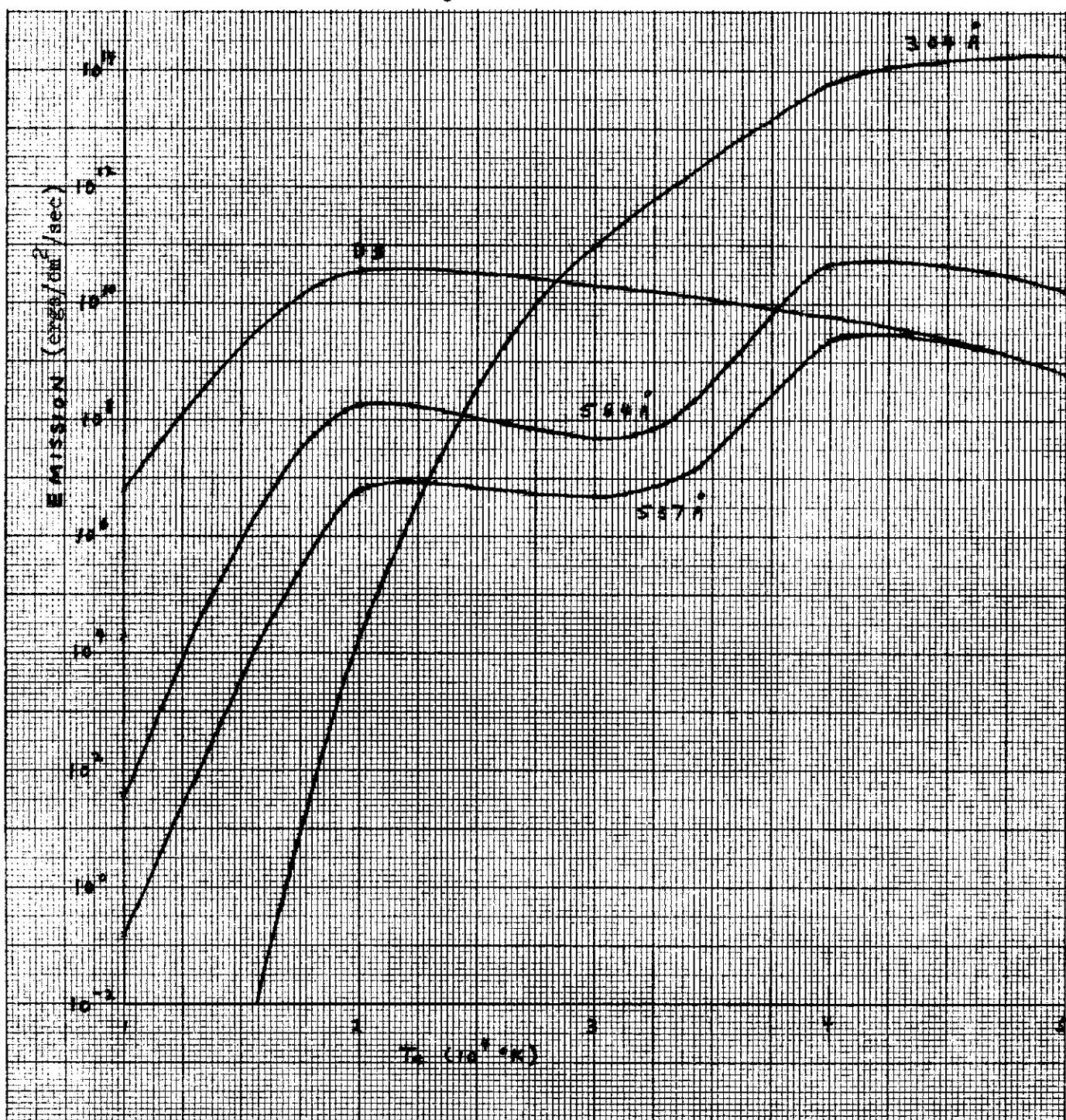


Figure II-35 TOTAL LINE EMISSION

$$T_e = 10^4 \text{ } ^\circ\text{K}$$

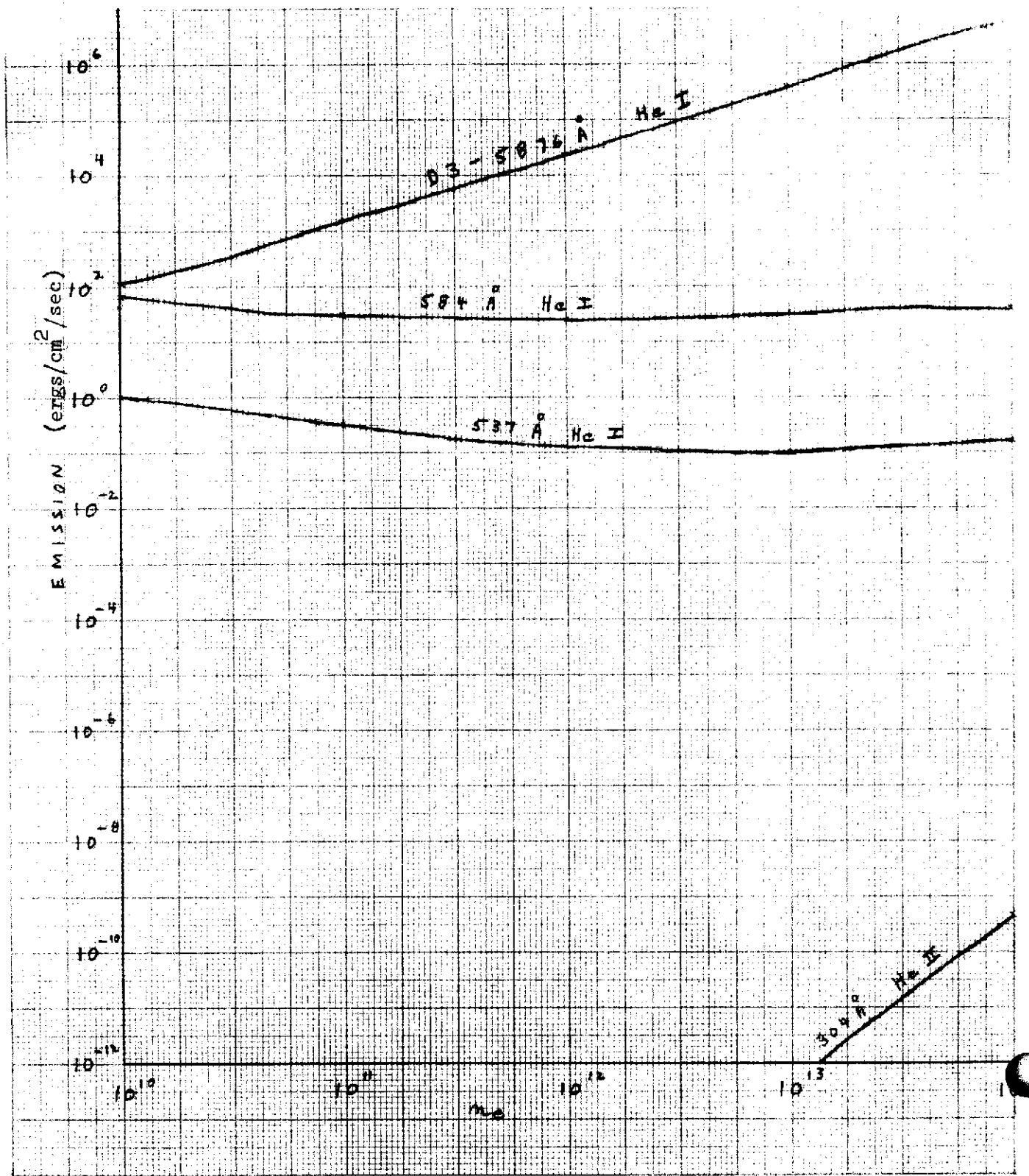


Figure II-36 TOTAL LINE EMISSION

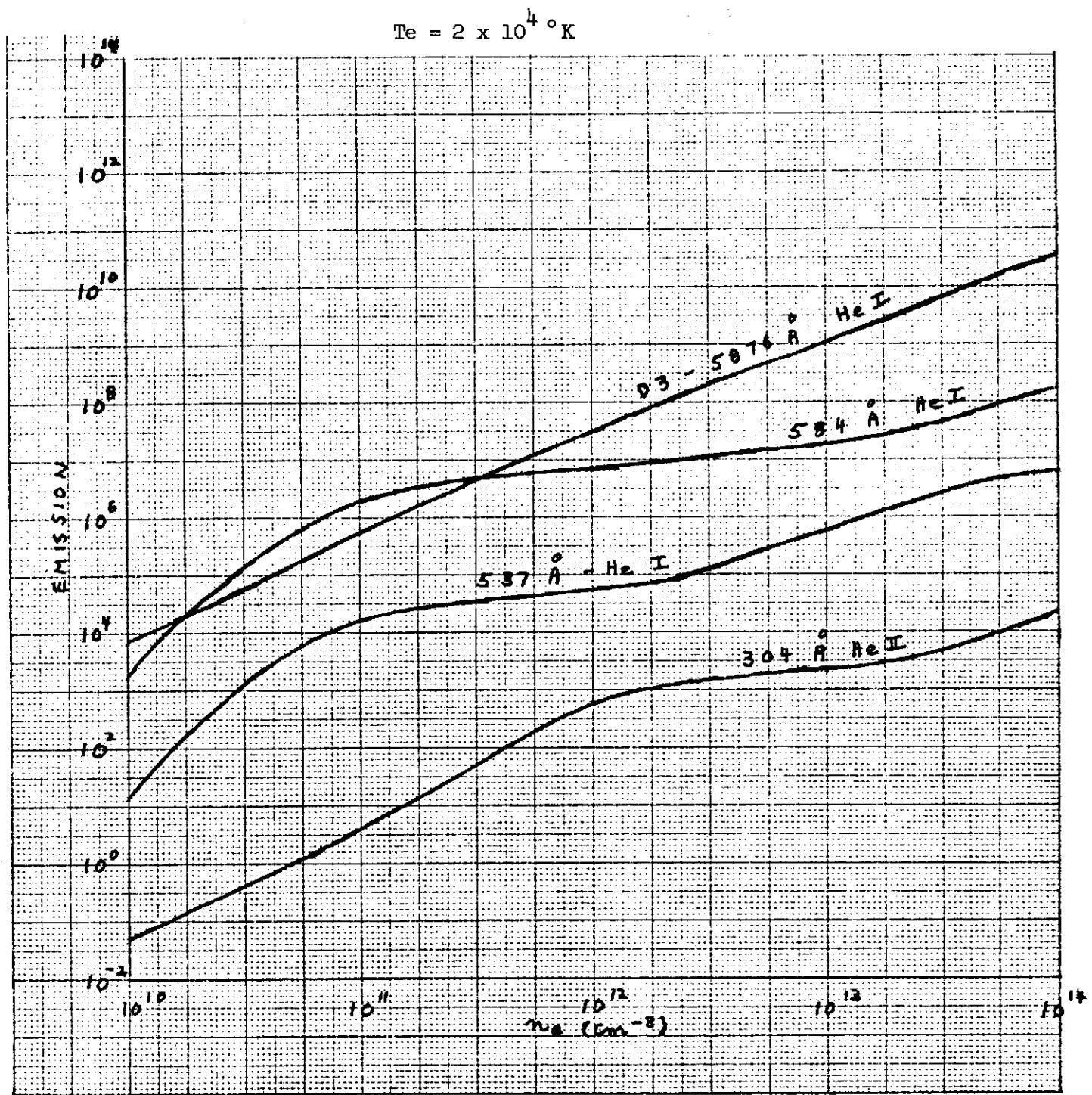


Figure II-37 TOTAL LINE EMISSION

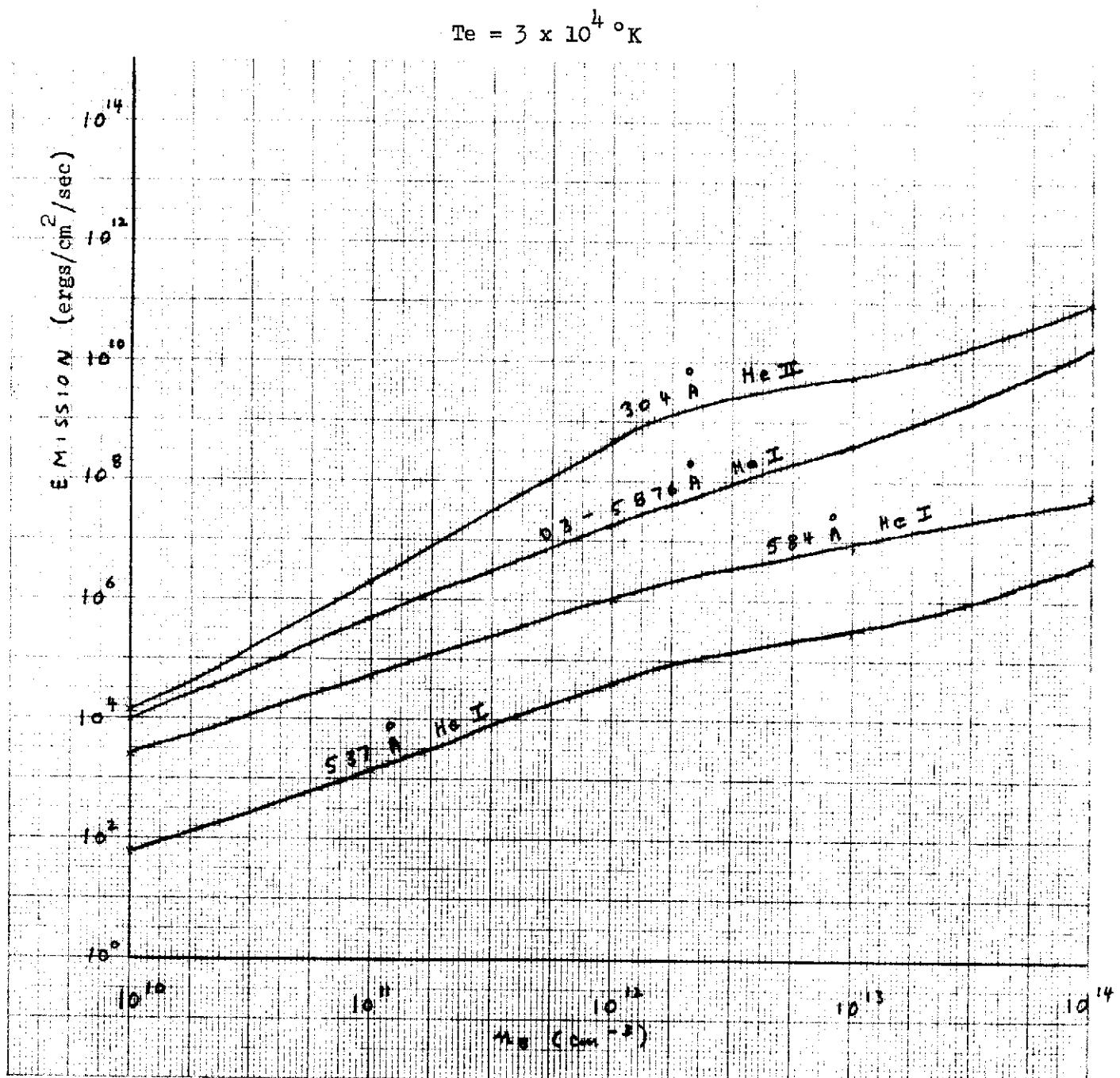


Figure II-38 TOTAL LINE INTENSITY

$$T_e = 4 \times 10^4 \text{ } ^\circ \text{K}$$

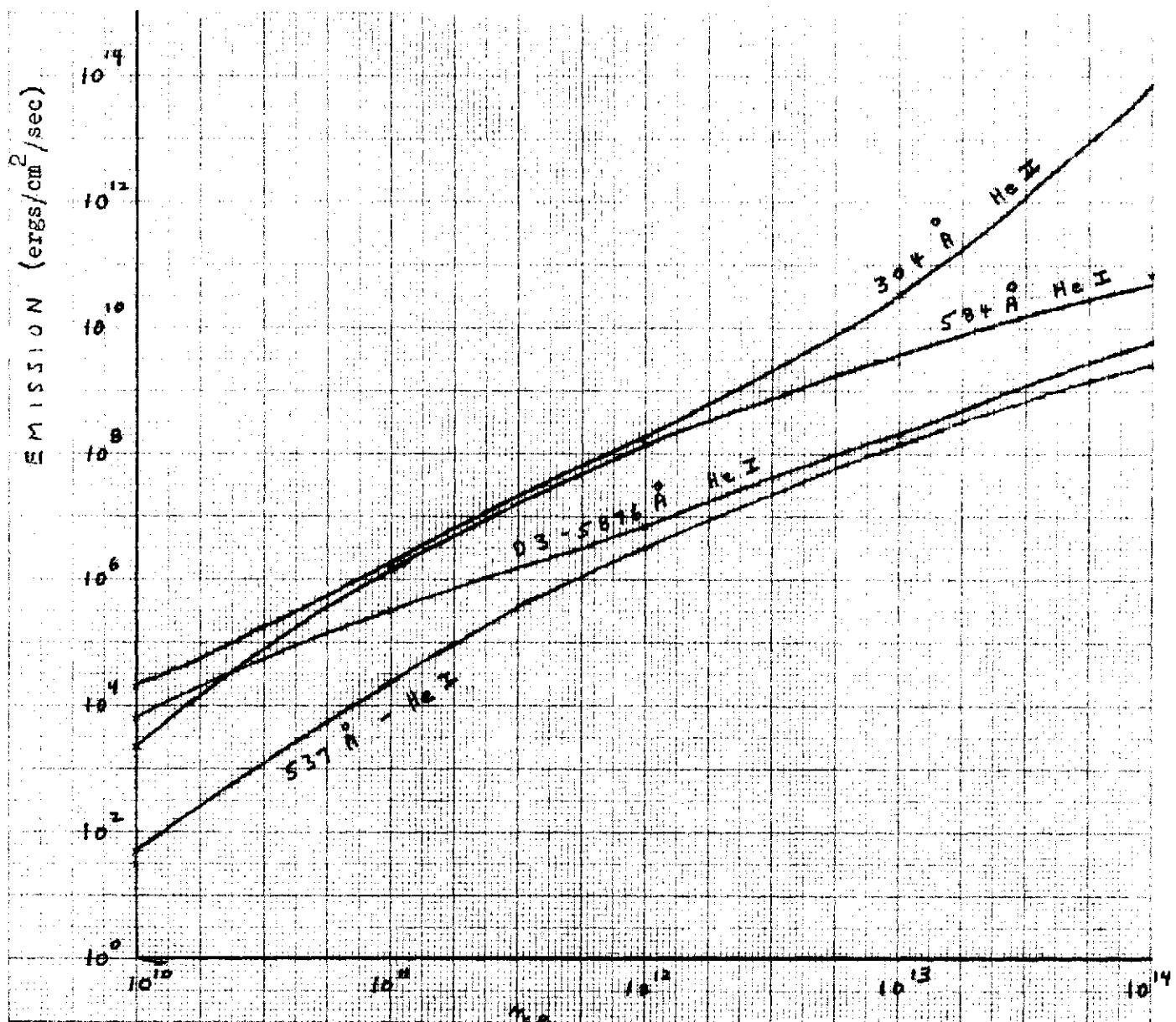
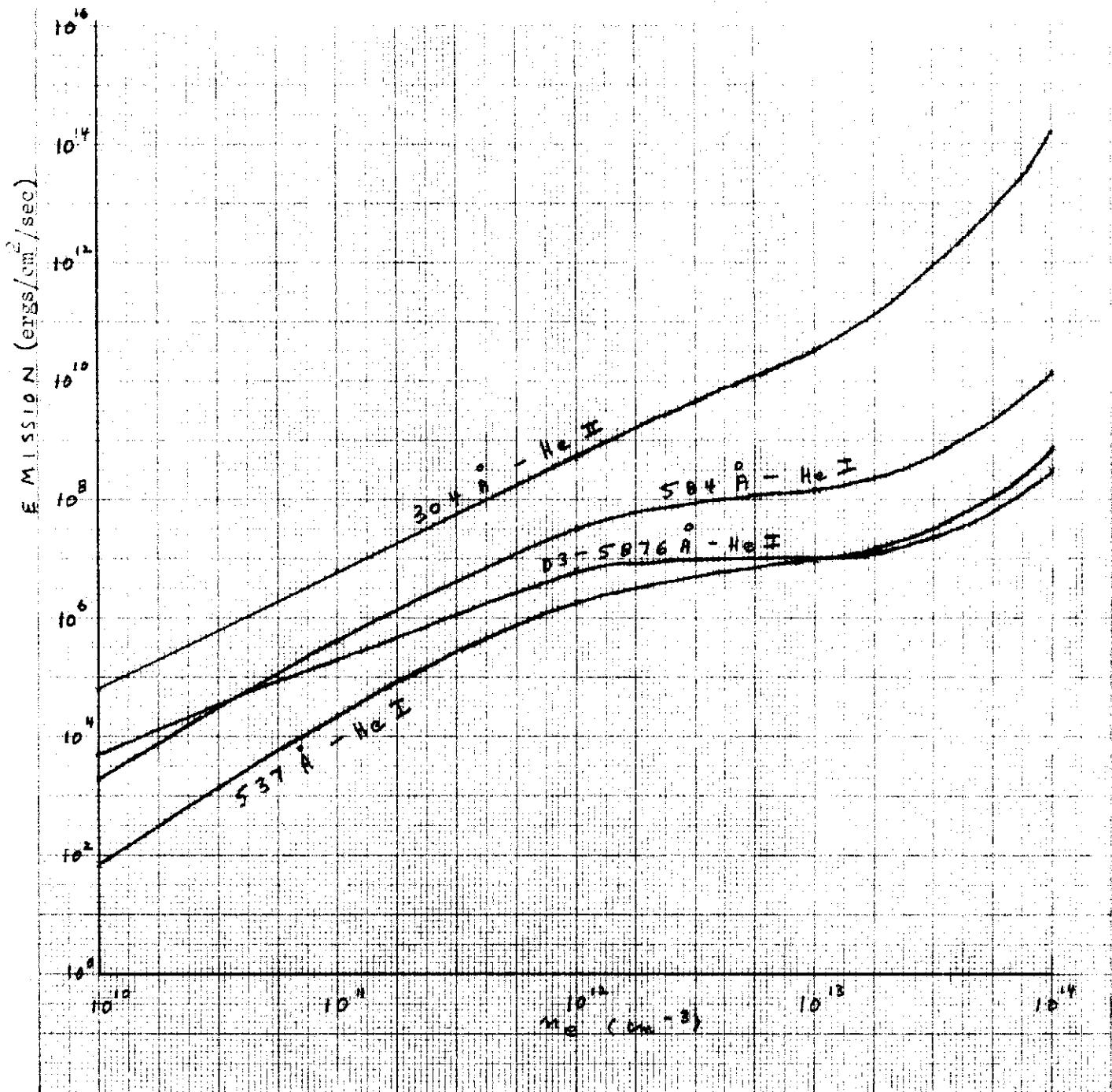


Figure II-39 TOTAL LINE EMISSION

 $T_e = 50,000^{\circ} \text{K}$ 

4. Population Rates

It is very instructive to look at the various processes involved in populating and depopulating the upper radiating levels. In other words, to determine the exact processes contributing significantly to the terms Π and ι in the transport equation. One way to do this is to assume a 3 or 4 level atom and evaluate Π and ι from the analytic solution choosing different levels for the 3rd or 4th levels. This would give us an approximate answer. Another way is to use the complete solution of the statistical equilibrium equations for the populations to evaluate the rates directly into the upper and lower levels of the lines in question.

Solutions of the full SSS equations were used in obtaining the relative rate processes shown in Figs. II-40 and II-41. Fig. II-40 illustrates the processes populating the 584 Å line upper level at $T_e = 40,000^{\circ}\text{K}$ for various electron densities. Four processes always enter significantly. The largest of these is photoexcitation from the 2¹S level by absorption of photospheric radiation. Direct collisional excitation from the ground state is next, followed by collisional excitation from the 2³S and radiative decay from the 3¹D. Hence, both the photospheric radiation and coupling to the triplet levels are important.

Fig. II-41 shows relative processes populating the D3 line upper level for the same electron temperature and densities. A much stronger dependence on n_e is noted. Photoabsorption of photospheric radiation in the D3 line itself is the dominant mechanism at low n_e . At high n_e , this process is small and the collisional rate from the 3¹D is dominant with collisional excitation from the 3³P and 2³S levels also being significant. Thus, the triplet - singlet interaction is again very important.

Figure II-40 RELATIVE PROCESSES POPULATING 2^1P LEVEL OF He I

$T_e = 40,000^\circ K$

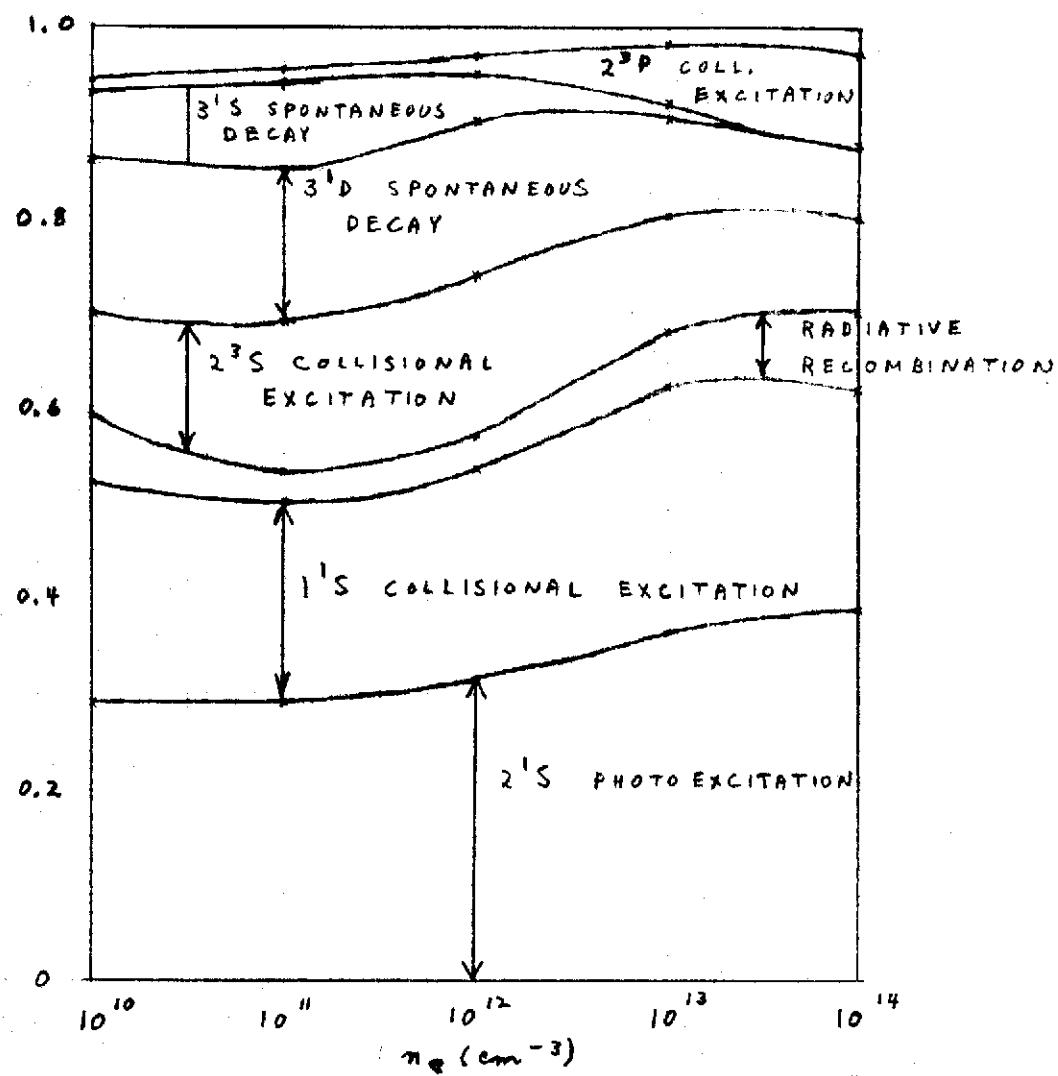
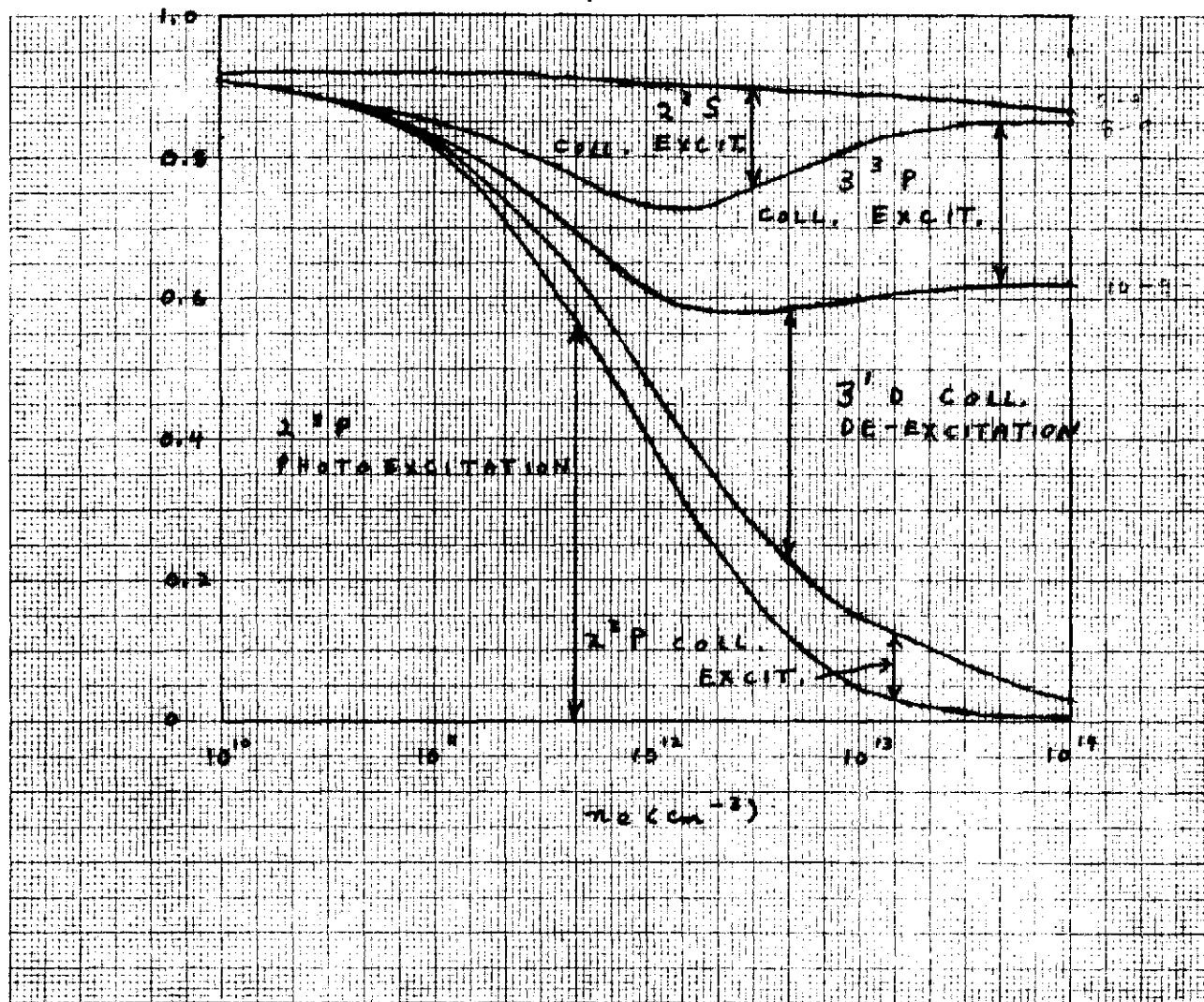


Figure II-41 RELATIVE RATES OF PROCESSES POPULATING THE $3^3 D$ LEVEL OF He I

$T_e = 40,000^\circ K$



III. LINE TRANSPORT SOLUTION

A. Basic Equations

The solution of the line transport equation that we have used in the code developed (Code 2) is an iterative solution of the integral equation. The details of the method have been developed by Avrett and Loeser (1969) in a manner convenient for the simultaneous solution of both line and continuum transport equations. From Section II.D, we note that solution for the line and continuum radiation field simultaneously is necessary. We will only briefly summarize the method and equations in this report.

In the statistically steady state the rate equation describing the population n_i of the state i is

$$\sum_{j \neq i} (n_j P_{ji} - n_i P_{ij}) = \sum_j n_j P_{ji} = 0$$

$$P_{ii} = - \sum_{j \neq i} P_{ij}, \quad \text{III.1}$$

where P_{ij} is the total transition rate from i to j per second per particle in the i state. In general, $P_{ij} = R_{ij} + C_{ij}$, where R_{ij} and C_{ij} represent the radiative and collisional transition rates respectively. We shall assume a Maxwellian distribution for the electrons and helium particles and since we also assume a known external radiation field, the transitions involving the continuum can be represented by a single term in Eq. III.1. We can characterize the system of linear equations III.1 by a matrix whose coefficients a_{ij} are equal to P_{ji} . In representing matrix elements and co-factors thereof, we shall always let the first subscript refer to the row and the second to the column. Because of the definition of the transition rate the subscripts of the P 's will be reversed when substituted for the matrix elements a . The general solution of Eq. III.1 is

$$n_i = \lambda_m^{mi}; \quad \lambda_m = \frac{N}{\sum_j P_{mj}}, \quad \text{III.2}$$

where P^{mj} is the co-factor of the element $a_{mj} = P_{jm}$ in the coefficient matrix represented by the i equations of type III.1 and N is the total number of helium particles per cm^3 . The matrix of coefficients has the property that the co-factor of all the elements in a column are equal, i.e. P^{mj} is independent of m .

When the medium becomes optically non-thin for certain frequencies the radiation field producing internal excitation and ionization for these frequencies is no longer merely the external radiation field but is partly dependent on the internal properties of the gas and must be determined from the radiative-transfer equation

$$\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu, \quad \text{III.3}$$

where $\cos^{-1}\mu$ represents the angle between the direction of propagation and the outward normal z and $\tau_\nu = \int k_\nu dz$, S_ν is the source function, k_ν is the linear absorption coefficient and I_ν is the specific intensity of the radiation. In LTE $S_\nu = B_\nu$, however in the non-LTE case S_ν must be specified in terms of microscopic processes. In terms of such processes the transfer equation governing the spectral line between upper level u and lower level l may be written as

$$-4\pi\mu \frac{dI_\nu}{dz} = [n_l B_{lu} \Phi_\nu h\nu - n_u B_{ul} \Psi_\nu h\nu + 4\pi k_c] I_\nu - n_u A_{ul} j_\nu h\nu - 4\pi k_c S_c(T_e), \quad \text{III.4}$$

where k_c represents the continuum absorption coefficient at frequency ν_0 and S_c is the continuum source function. B_{lu} , B_{ul} and A_{ul} are the Einstein transition probabilities for absorption, stimulated emission and spontaneous emission. j_ν , Ψ_ν and Φ_ν are the normalized emission, stimulated emission and absorption coefficients within the line defined such that

$$\int_0^\infty \Phi_\nu d\nu = \int_0^\infty \Psi_\nu d\nu = \frac{1}{4\pi} \int_{4\pi}^\infty \int_0^\infty j_\nu d\nu dw = 1.$$

The continuum absorption coefficient is generally very small compared with the line absorption coefficient near the line center and will be neglected in determining the source function within the line. Using the standard relations between the Einstein coefficients and assuming $j_\nu = \Phi_\nu = \Psi_\nu$, the source function becomes

$$S_{ul} = \frac{2h\nu^3}{c^2} \frac{1}{[(g_u/g_l)(n_l/n_u)]-1}, \quad \text{III.5}$$

where g represents the statistical weight. The minus one term in the denominator represents stimulated emissions.

In evaluating the radiative excitation rate R_{ij} for transitions between bound levels the line radiation field enters as

$$\int_0^\infty J_\nu(\tau) \Phi_\nu(\tau) d\nu = \bar{J}(\tau)$$

where

$$J_\nu(\tau) = \frac{1}{4\pi} \int_{4\pi} I_\nu(\tau, \mu) d\omega$$

is the mean intensity and $d\omega$ represents the solid angle. It is thus convenient to formulate the transfer equation in terms of J_ν rather than I_ν . It is now convenient to separate those components involving the unknown radiation field, J_{ul} , from the co-factors. This is done by expanding the determinant P^{ij} in terms of its co-factors Q^{ij} . Thus

$$P^{lu} = \sum_{k \neq l} P_{lk} Q^{kl} = P_{lu} Q^{ul} + \sum_{k \neq l \neq u} P_{lk} Q^{kl} \quad \text{III.6}$$

$$P^{ul} = \sum_{k \neq u} P_{uk} Q^{ku} = P_{ul} Q^{lu} + \sum_{k \neq u \neq l} P_{uk} Q^{ku}.$$

Actually, J_{ul} may appear in many of the co-factors since the line $u-l$ may fall in the ionization continuum of some other transition. The influence of J_{ul} as well as the line radiation in general on the bound-free radiative rates will be neglected. Using the standard relationship between the

Einstein coefficients, equation III.6, and remembering that $Q_{ul}^{ul} = Q^{lu}$ and $A_{lu} = B_{lu} \int J_v \Phi_v dv$ the source function may be written as

$$S_{ul} = \rho_{ul} \frac{P_{lu}}{P_{ul}} = \frac{\int_{ul} J_v \Phi_v dv + \epsilon B + \zeta}{1 + \epsilon + \eta} \quad \text{III.7}$$

where B is the Planck function

$$B_v(T_e) = \rho_{ul} \frac{C_{lu}}{C_{ul}}$$

$$\epsilon = \frac{C_{ul}}{A_{ul}} \quad \rho_{ul} = \frac{2h\nu^3}{c^2} \frac{g_l}{g_u}$$

$$\zeta = \rho_{ul} \frac{1}{A_{ul} Q^{ul}} \sum_{k \neq u \neq l} P_{lk} Q^{kl} \quad \text{III.8}$$

$$\eta = \frac{1}{A_{ul} Q^{ul}} \sum_{k \neq u \neq l} P_{uk} Q^{ku}$$

The terms entering the numerator of Eq. III.7 each represent a method of populating the upper level from the lower level. The first term represents direct radiative excitation, the second direct collisional excitation and the third any combination of radiative or collisional processes involving one or more intermediate levels in going from the lower to the upper level. The denominator, on the other hand, consists of terms indicating transition paths from the upper to the lower level. All the terms are normalized with respect to A_{21} . The first term represents direct radiative de-excitation, the second direct collisional de-excitation and the third any indirect process going from the upper to the lower state.

Equation III.7 is solved using a discrete ordinate method for the frequency integral in which we assume

$$\int_0^\infty F(x) dx = \sum_{k=1}^K A_k F_k. \quad \text{III.9}$$

The coefficients are to be found from a given set of dimensionless frequency values x_k , $k = 1, 2, \dots, K$; F_k is the value of F at $x = x_k$. The solution for A_k is given in Section III.C.

We shall assume Φ_ν to be Gaussian, i.e.

$$\Phi_\nu = \frac{\exp(-v^2)}{(\pi)^{1/2} \Delta\nu_D}; \quad v = \frac{\Delta\nu}{\Delta\nu_D}. \quad \text{III.10}$$

$\Delta\nu_D$ is the Doppler half width given by

$$\frac{\nu_0}{c} \left(\frac{2kT}{M} \right)^{1/2} \quad \text{III.11}$$

where M is the Helium particle mass.

The source function is obtained at N depth points ($i = 1 \dots N$) within the assumed layer. The depth points are located at specified physical depths which do not change during the calculation. The values of S_i are obtained from the matrix equation

$$\sum_{j=1}^N M_{ij} S_j = C_i \quad \text{III.12}$$

where i and j refer to depth points.

The coefficients M_{ij} are given by

$$M_{ij} = \Delta_{ij} - \frac{1}{1+\epsilon_i} \bar{W}_{ij}^{(\Lambda)} \quad \text{III.13}$$

where

$$\Delta_{ij} = \begin{cases} 1, & j = i \\ 0, & j \neq i \end{cases}$$

$w_{ij}^{(\Lambda)}$ are weighting functions, ϵ' is a coupling parameter.

c_j are given by

$$c_j = \frac{\epsilon'_i}{1+\epsilon'_i} B_i^S - \frac{1}{1+\epsilon'_i} \sum_{j=1}^N w_{ij}^{(\Lambda)} S_j^C \quad III.14$$

In these equations, B_i^S is a coupling parameter,

$$\bar{w}_{ij}^{(\Lambda)} = \frac{2}{\sqrt{\pi}} \sum_{k=1}^K A_k w_{ijk}^{(\Lambda)} \frac{\phi_{ik} \phi_{jk}}{\phi_{ik} + r_j} \quad III.15$$

and

$$w_{ij}^{(\Lambda)} = \frac{2}{\sqrt{\pi}} \sum_{k=1}^K A_k \bar{w}_{ijk}^{(\Lambda)} \frac{\phi_{ik} r_i}{\phi_{jk} + r_j} \quad III.16$$

where k refers to a specific frequency, A_k are weighting functions. The profile function ϕ_{ik} is simply

$$\phi_{ik} = e^{-v_k^2}$$

The optical depth values τ_{ik} are given by

$$\tau_{ik} = \int_0^{\tau_i} (\phi_{ik} + r_i) d\tau$$

$$d\tau = k^L dz$$

$$k^L = \frac{h v_o}{4\pi^{3/2} \Delta \omega_D} n_1 B_{12}$$

The weighting coefficients $w_{ijk}^{(\Lambda)}$ represent an expansion of the mean intensity $J_v(\tau_{vi})$ in terms of the source function $S_v(\tau_{vj})$

$$J_v(\tau_{vi}) = \sum_{j=1}^N w_{ijk}^{(\Lambda)} S_v(\tau_{vj}) \quad \text{III.17}$$

Substituting the solution of the radiative transport equation for J_v we obtain

$$\frac{1}{\pi} \int_0^{T_1} E_1(|t-\tau_i|) S(t) dt = \sum_{j=1}^N w_{ij}^{(\Lambda)} S(\tau_i) \quad \text{III.18}$$

where the frequency subscript has been dropped. To evaluate $w_{ij}^{(\Lambda)}$ we assume that S_i is represented by linear segments between optical depth points n and $n+1$. $S(t)$ in the interval $n \leq t \leq \tau_{n+1}$ is given by

$$S(t) = S_n \left(\frac{\tau_{n+1} - t}{\tau_{n+1} - \tau_n} \right) + S_{n+1} \left(\frac{t - \tau_n}{\tau_{n+1} - \tau_n} \right) \quad \text{III.19}$$

Equations for $w_{ij}^{(\Lambda)}$ are obtained by substituting Eq. III.19 into Eq. II.18.

The $w_{ij}^{(\Lambda)}$ so obtained depend only on the set of τ_i values chosen. Different expressions for $w_{ij}^{(\Lambda)}$ are obtained for $j > i$, $j < i$, and $j = i$. We give these expressions in order.

$w_{ij}^{(\Lambda)}$ depends only on the coefficient of S_n

$$2w_{in} = \int_{\tau_{n-1}}^{\tau_n} E_1 |t-\tau_i| \frac{(t-\tau_{n-1})dt}{\tau_n - \tau_{n-1}} + \int_{\tau_n}^{\tau_{n+1}} E_1 |t-\tau_i| \frac{(\tau_{n+1}-t)}{\tau_{n+1} - \tau_n} dt.$$

III.20

For $n > i$,

$$2W_{in} = \left[\frac{\tau_i(E_2|\tau_{n-1}-\tau_i| - E_2|\tau_n-\tau_i|) + e^{-|\tau_{n-1}-\tau_i|} - e^{-|\tau_n-\tau_i|} + E_3|\tau_n-\tau_i| - E_3|\tau_{n-1}-\tau_i|}{(\tau_n - \tau_{n-1})} \right.$$

$$- \frac{\tau_{n-1}}{\tau_n - \tau_{n-1}} [E_2|\tau_{n-1}-\tau_i| - E_2|\tau_n-\tau_i|] + \frac{\tau_{n+1}}{\tau_{n+1}-\tau_n} [E_2|\tau_n-\tau_i| - E_2|\tau_{n+1}-\tau_i|]$$

$$\left. - \frac{\tau_i(E_2|\tau_n-\tau_i| - E_2|\tau_{n+1}-\tau_i|) + e^{-|\tau_n-\tau_i|} - e^{-|\tau_{n+1}-\tau_i|} + E_3|\tau_{n+1}-\tau_i| - E_3|\tau_n-\tau_i|}{(\tau_{n+1}-\tau_n)} \right].$$

III.21

For $n < i$,

$$2W_{in} = \frac{(\tau_i - \tau_{n-1})}{(\tau_n - \tau_{n-1})} [E_2(\tau_i - \tau_n) - E_2(\tau_i - \tau_{n-1})] + \frac{(\tau_{n+1} - \tau_i)}{(\tau_{n+1} - \tau_n)} [E_2(\tau_i - \tau_{n+1}) - E_2(\tau_i - \tau_n)]$$

$$+ [e^{-(\tau_i - \tau_{n+1})} - e^{-(\tau_i - \tau_n)} + E_3(\tau_i - \tau_n) - E_3(\tau_i - \tau_{n+1})]/(\tau_{n+1} - \tau_n)$$

$$- [e^{-(\tau_i - \tau_n)} - e^{-(\tau_i - \tau_{n-1})} + E_3(\tau_i - \tau_{n-1}) - E_3(\tau_i - \tau_n)]/(\tau_n - \tau_{n-1}).$$

III.22

For $i = n$,

$$2W_{in} = \frac{(\tau_i - \tau_{n-1})}{(\tau_n - \tau_{n-1})} [1 - E_2(\tau_i - \tau_{n-1})] + \frac{(\tau_{n+1} - \tau_i)}{(\tau_{n+1} - \tau_n)} [1 - E_2(\tau_{n+1} - \tau_i)]$$

$$- \frac{[1/2 - e^{-(\tau_i - \tau_{n-1})} + E_3(\tau_i - \tau_{n-1})]}{\tau_n - \tau_{n-1}} - \frac{[1/2 - e^{-(\tau_{n+1} - \tau_i)} + E_3(\tau_{n+1} - \tau_i)]}{\tau_{n+1} - \tau_n}$$

III.23

B. Evaluation of ϵ' and B^S

ϵ' and B^S appearing in Eqs. III.13 and III.14 are related to the source function parameters ϵ , η and ζ as follows:

$$\begin{aligned}\epsilon' B^S &= \epsilon B + \zeta \\ \epsilon' &= \epsilon + \eta\end{aligned}\quad \text{III.24}$$

where B is the Planck function. The values of ϵ' and B^S depend upon the levels included in the model other than the upper and lower line levels.

For two bound levels (1,2) and one continuum level (k) ϵ' and $\epsilon' B^S$ are given by:

$$\epsilon' = \frac{c_{21}}{A_{21}} (1 - \beta) + \frac{\bar{P}_{21}}{A_{21}} - \frac{\omega_1}{\omega_2} \frac{\bar{P}_{12}}{A_{21}} \quad \text{III.25}$$

$$\epsilon' B^S = \frac{c_{21}}{A_{21}} (1 - \beta) B + \alpha \frac{\omega_1}{\omega_2} \frac{\bar{P}_{12}}{A_{21}}$$

where $\alpha = \frac{2h\nu_{21}^3}{c^2}$, $\beta = e^{-h\nu_{21}/kT}$

III.26

$$\bar{P}_{ij} = P_{ik} P_{kj} / (P_{ki} + P_{kj})$$

For three bound levels and a continuum level

$$\begin{aligned}\epsilon' &= X - Y \\ \epsilon' B^S &= \alpha Y\end{aligned}\quad \text{III.27}$$

where

$$X = \frac{1}{A_{21}} (c_{21} + \bar{P}_{21} + P_{23} + \bar{P}_{23} - \frac{M_{12} M_{21}}{M_{22}}) \quad \text{III.28}$$

$$Y = \frac{1}{A_{21}} \frac{\bar{\omega}_1}{\omega_2} (C_{12} + \bar{P}_{12} - \frac{M_{12} R_2}{M_{22}}) \quad III.29$$

$$M_{12} = P_{32} + \bar{P}_{32}$$

$$M_{21} = P_{23} + \bar{P}_{23}$$

$$M_{22} = P_{31} + \bar{P}_{31} + P_{32} + \bar{P}_{32}$$

$$R_2 = P_{13} + \bar{P}_{13}$$

III.30

For some applications it is convenient to solve for two line radiation fields simultaneously using only the four levels in Code 2. The two lines are then represented by the 3 - 1 and 2 - 1 transitions. The corresponding X and Y values for the 3 - 1 lines are

$$X = \frac{1}{A_{31}} (C_{31} + \bar{P}_{31} + P_{32} + \bar{P}_{32} - \frac{M_{12} M_{23}}{M_{11}}) \quad III.31$$

$$Y = \frac{1}{A_{31}} \frac{\bar{\omega}_1}{\omega_3} (C_{13} + \bar{P}_{13} - \frac{M_{21} R_1}{M_{11}})$$

where

$$M_{11} = P_{21} + \bar{P}_{21} + P_{23} + \bar{P}_{23} \quad III.32$$

$$R_1 = P_{12} + \bar{P}_{12}$$

In the general case ϵ' and B^S are obtained from Code 1 at each optical depth. Code 1 can be run for arbitrary values of \bar{J} for the lines or \bar{A} for the continuum rates.

C. Evaluation of A_k

The evaluation of A_k follows that of Avrett and Loeser (1969) which is recommended for further details. $F_k(x)$ is represented by

$$F_k = \sum_{j=1}^K f(x_k)_j c_j \quad 0 \leq x \leq x_K$$

where

III.33

$$f(x)_j = 1, \quad 0 \leq x \leq x_K$$

when $j = 1$, and

$$f(x)_j = \begin{cases} (1 - \frac{x}{x_j}) (1 - y \frac{x}{x_j}), & 0 \leq x \leq x_j \\ 0, & x_j \leq x \leq x_K \end{cases} \quad III.34$$

when $j = 2, 3, \dots, K$. y is an adjustable parameter.

A_k is given by

$$A_k = \sum_{j=1}^K g_j f_{jk}^{-1} \quad III.35$$

where f_{jk}^{-1} is the inverse of $f(x_k)_j$ and

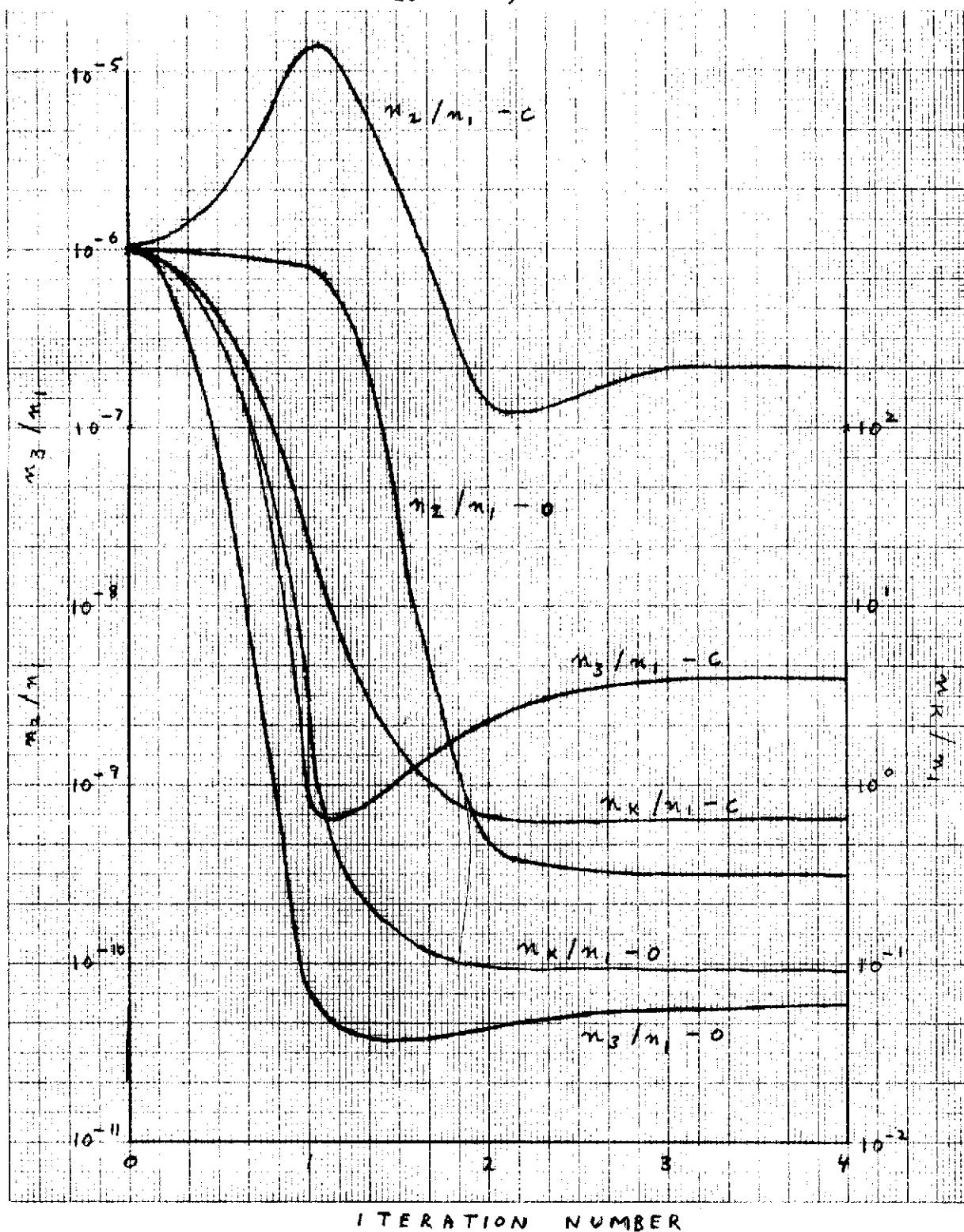
$$g_j = \begin{cases} x_K, & j = 1 \\ \frac{1}{2} x_j (1 - \frac{y}{3}), & j = 2, 3, \dots, K. \end{cases} \quad III.36$$

D. Sample Solution - Two Lines

The inputs to code 2 to begin the iterative solution are the n_j/n_1 . Approximate starting values are obtained from code 1. We shall illustrate the solution by discussing the populations n_2/n_1 , n_3/n_1 and n_K/n_1 , where 1, 2 and 3 designate the lower level and two upper line levels for which the transport equations are solved and K the continuum level. ϵ_i and B_i^S are obtained as described in Section III.B. n_1 and the optical depths at the geometric depth points are calculated by the code from the given population ratios and n_{TOTAL} . For the initial run, the upward radiative rates are those given by the optically thin case. S_j values are calculated from Eq. III.12. \bar{J}_j is found from the S_j and the new radiative excitation rate based on \bar{J}_j is used to obtain new values of n_j/n_1 through code 1 or a simpler 3 or 4 level solution. The new values of n_j/n_1 and \bar{J} are used as input to code 2 (or 3) to obtain the other line intensity.

We illustrate the solution for two lines in Fig. III-1 for $T_e = 2 \times 10^4$ °K and $n_e = 10^{12}$ cm⁻³. The Figure shows results for n_2/n_1 , n_3/n_1 and n_K/n_1 as a function of the number of iterations. The initial values of n_2/n_1 and n_3/n_1 are 10^{-6} and n_K/n_1 is 10^2 . The solutions have essentially converged after 2-3 iterations. Solutions at the surface of the layer are labeled -0; solutions at the center of the layer are labeled -C. The codes have been tested for a number of simultaneous line and continuum transfer problems. There have been no convergence difficulties provided the lines and continua chosen for solution do significantly effect each other.

Figure III-1 2 LINE SOLUTION - CONVERGENCE

 $T_e = 20,000^{\circ}\text{K}$ 

IV. CONTINUUM TRANSPORT SOLUTION

A. Basic Equations

The statistical equilibrium equation for one bound level (n_1) and one continuum level (n_k) is

$$\frac{n_1}{n_1^*} \left[4\pi \int_{v_1}^{\infty} \frac{a_v}{hv} J_v dv + C_{lk} \right] = \frac{n_k}{n_k^*} \left[4\pi \int_{v_1}^{\infty} \frac{a_v}{hv} e^{-hv/kT} \left(\frac{2hv^3}{c^2} + J_v \right) dv + C_{lk} \right], \quad IV.1$$

where the * refers to the LTE population at a given electron temperature and density. It is convenient to express the population ratio n_1/n_k in terms of the non-equilibrium parameter b_1 ,

$$b_1 = (n_1/n_1^*) / (n_k/n_k^*). \quad IV.2$$

The radiative transport equation for $v > v_1$ can be written

$$\mu \frac{dI_v}{d\tau_v} = I_v - \frac{B_v^*}{b_1} \quad IV.3$$

where neglecting stimulated recombination (which is justified for He for the temperatures considered)

$$B_v^* = \frac{2hv^3}{c^2} e^{-hv/kT}$$

$$d\tau_v = k_v dz \quad IV.4$$

$$k_v = n_1 a_v$$

The values of b_{li} at depth i are found by solving the set of equations

$$\sum_{j=1}^N M_{ij} \frac{1}{b_{ij}} = \frac{\epsilon_i^b}{\epsilon_i^a} \quad i = 1, 2, \dots, N \quad IV.5$$

where

$$M_{ij} = \Delta_{ij} - \frac{1}{\epsilon_i^a R_i^a} \sum_{k=1}^K A_k' w_{ijk}^{(\Lambda-1)} \frac{g_k}{y_k} e^{-y_k \theta_j} \quad IV.6$$

$$\Delta_{ij} = \begin{cases} 1, & j = i \\ 0, & j \neq i \end{cases}$$

and

$$R_i^a = \sum_{k=1}^K A_k' \frac{g_k}{y_k} e^{-y_k \theta_i} \quad IV.7$$

τ_i is the optical depth at the continuum threshold at depth i , $\theta_i = h\nu_1/kT_i$, $y_k = \nu_k/\nu_1$, $k = 1, 2, \dots, K$, a set of dimensionless frequency values and g_k are values such that $g_k y_k^{-3}$ represents the frequency dependence of the photo-ionization cross section. The optical depth is given by

$$\tau_{ik} = \frac{g_k}{g_1} \frac{1}{y_k^3} \tau_i \quad IV.8$$

ϵ_i^a and ϵ_i^b are coupling parameters whose calculation is described in the next section. The values of $w_{ijk}^{(\Lambda-1)}$ are related to $w_{ijk}^{(\Lambda)}$ as follows,

$$w_{ijk}^{(\Lambda-1)} = \begin{cases} w_{ijk}^{(\Lambda)} - 1, & j = 1 \\ w_{ijk}^{(\Lambda)}, & j \neq i. \end{cases} \quad IV.9$$

The mean intensity of the radiation field is given by

$$J_{ik} = \sum_{j=1}^N w_{ijk}^{(\Lambda)} \frac{B_{jk}^*}{b_{ij}} \quad IV.10$$

B. Evaluation of ϵ_i^a and ϵ_i^b

ϵ_i^a and ϵ_i^b follow from the statistical equilibrium equation solution for b_1 ,

$$\frac{1}{b_1} = \frac{(R_{1k}/R_{1k}^*) + \epsilon^b}{1 + \epsilon^a} \quad \text{IV.11}$$

where

$$R_{1k} = 4\pi \int_{v_1}^{\infty} \frac{a_v}{hv} J_v dv \quad \text{IV.12}$$

$$R_{1k}^* = 4\pi \int_{v_1}^{\infty} \frac{a_v}{hv} B_v dv.$$

For two bound levels (1,2) and a continuum level k, ϵ_i^a and ϵ_i^b are

$$\epsilon^b = \frac{1}{R_{1k}^*} (c_{1k} + \frac{P_{12} P_{2k}}{P_{21} + P_{2k}}) \quad \text{IV.13}$$

$$\epsilon^a = \frac{1}{R_{1k}^*} (c_{1k} + \frac{(n_2^*/n_1^*) P_{21} (n_k^*/n_2^*) P_{k2}}{P_{21} + P_{2k}}).$$

For an N level model the corresponding equations are

$$\epsilon^b = \frac{1}{R_{1k}^*} (c_{1k} + \frac{1}{Q^{kl}} \sum_{l \neq 1 \neq k}^N P_{1l} Q^{\ell l})$$

$$\epsilon^a = \frac{1}{R_{1k}^*} (c_{1k} + \frac{1}{Q^{lk}} \sum_{l \neq 1 \neq k}^N P_{kl} Q^{\ell k}). \quad \text{IV.14}$$

ϵ^a and ϵ^b can easily be obtained from program 1.

C. Evaluation of A'_k

The A'_k coefficients are defined such that

$$\int_1^{y_k} F(y) dy = \sum_{k=1}^K A'_k F_k \quad IV.15$$

where F_k is the value of F at $y = y_k$. Here, $1 \leq y_k \leq y_K$. With unity instead of zero as the lower integration limit, we determine the A'_k coefficients as follows.

Let $f'(y)_j = 1$, $1 \leq y \leq y_k$,

when $j = 1$, and

$$f'(y)_j = \begin{cases} (1 - \frac{y-1}{y_j-1}) (1 - y \frac{y-1}{y_j-1}), & 1 \leq y \leq y_j \\ 0, & y_j \leq y \leq y_K, \end{cases} \quad IV.16$$

when $j = 2, 3, \dots, K$. Let f'_{jk}^{-1} be the inverse of $f'(y_k)_j$. Then

$$A'_k = \sum_{j=1}^K g'_j f'_{jk}^{-1}, \quad IV.17$$

where

$$g'_j = \begin{cases} y_K^{-1}, & j = 1 \\ \frac{1}{2} (y_j^{-1})(1 - \frac{Y}{3}), & j = 2, 3, \dots, N. \end{cases} \quad IV.18$$

Y is an adjustable parameter.

V. CODES

A. Code 1 - Solution of Statistically Steady State Population Equations

1. Main Program

In our own internal notation, this code is designated as P48. The main program reads f numbers, wavelengths (λ), electron and radiation temperatures, the energy level model, recombination coefficients, converts energy differences from wave numbers to electron volts, and writes all the above before entering subroutine CONSTS. The subroutine CONSTS as well as other subroutines are described in the next section. The radiation temperature is that characterizing the external Blackbody radiation field incident upon the layer. The indices on the f numbers refer to the ion and the upper and lower line levels respectively.

On return to the main program, more quantities are read in and printed out, such as: the total line center optical depth of the layer, the dilution factor for the external radiation, the electron density, the indeces of the chosen thick line, the depth points at which solutions are to be obtained, a constant divisor for the elements of the main matrix to prevent overflow, Y values for thick lines, and various control numbers. These quantities are entered here in order to be able to run a series of different solutions by changing any or all of them without changing the electron or radiation temperatures and, thereby, having to recalculate the many reaction rates.

After the above have been printed and the ratio of B_o/B_{T_r} calculated the subroutine AMAT is entered to calculate the elements and cofactors of the A matrix for the optically thin case. The rate equation matrix represented by Eq. II-3 is printed out. The matrix is 30 x 30 corresponding to the number of energy levels. Selected cofactors are printed out. The accuracy of the solution can be checked by comparison of cofactors with the same j values.

The solution for the non-equilibrium populations n_1 is obtained in AMAT. The solutions are printed for the optically thin case along with LTE solutions for the same temperature and density. The optical depth at the center of each line is calculated and printed out for a layer of optical thickness T_1 in the line specified in the input. Some further quantities such as the physical thickness of the layer H are calculated and the subroutine ELIM is entered to compute ϵ , η and ζ .

The program now repeats the calculation with the specified set of Y values read in. Next, a DO loop on depth is set up. In the listing given there is no depth variable. In calling for one to obtain values of η and ζ for example, it would enter into the calculation of the quantity FF, which is used to alter the Y value for the thick line.

2. Description of Sub-Programs

Subroutine AMAT(KK)

AMAT calculates elements of the A matrix using quantities determined by CONSTS. Once all the elements are found, they are divided by a constant to prevent overflow. Cofactors are calculated, summed, and used to determine λ . From this the n_i are found. Next the n_{eqi} are found and the ratio n_i/n_{eqi} . Last, before returning to the main program, the optical depths are calculated and printed for each f value.

KK = 0 , optically thin solution

KK = 1 , optically thick solution for any Y ≠ 0.0.

Function COFACT (NR, NC, NE, D)

COFACT finds the cofactor of matrix D for row NR, column NC. NE is the number of rows and columns in D.

Function COLL (T, I, J, K, N)

Function C \emptyset LL calculates certain electron collisional excitation and ionization coefficients for special points.

T = electron temperature ($^{\circ}$ K)

I, J, K = indeces of coefficient

N = 1 , excitation coefficient calculated

N = 2 , ionization coefficient calculated

Subroutine CONSTS

Initially, if the radiation temperature is different from the electron temperature, CONSTS reads in new values of β_{ijk} calculated at T_r . It then calculates the electron collisional ionization and recombination coefficients, the radiative ionization rate, the B_{ijk} and B_{ikj} , the electron collisional excitation coefficient, the Einstein spontaneous transition probability, and the Einstein absorption transition probability multiplied by the Planck function. The subscript i refers to the ion, the second subscript the beginning level and the last subscript the ending level of the transition.

Subroutine ELIM (RHO, AP)

AP = Einstein spontaneous transition probability for the thick
line (K7, K8, K9)
RHO = $h\nu^3/c^2$, where ν is calculated at (K7, K8, K9)

This computes double cofactors for use in calculating eta and iota.
It is called from the main program and uses the function ELM2.

Function ELM2 (IRA, ICA, KRA, KCA, RMAT, Z)

IRA = row index of 1st row to be eliminated
ICA = column index of 1st column to be eliminated
KRA = row index of second row to be eliminated
KCA = column index of second column to be eliminated
RMAT = contains reduced matrix
Z = sign of cofactor ($Z = \pm 1$).

ELM2 eliminates two rows and two columns from the A matrix and places
the reduced matrix in RMAT.

B. Radiative Transfer Codes

Two codes have been developed under this program. The first (code 2) represents a numerical solution of the line transport equation given in Section III. The second (code 3) represents a numerical solution of the continuum transport equation. Listings of these codes appear in Appendices B and C. The simultaneous solution of several line and/or continuum transport eqs. with the population eqs. is accomplished by iteration. Initial values for population ratios are estimated from various solutions obtained from code 1 (see Section II). After obtaining the radiation intensities from codes 2 and 3 the new radiative rates are used as input to code 1 to obtain new population ratios to be used in the next iteration.

Code 2 requires the specification of certain quantities involving ϵ_i^r and B_i^S while code 3 requires ϵ_i^a and ϵ_i^b . There are two methods provided for determining these quantities. One option is to calculate them in code 1 and simply read them in. (Code 1 is now set up to calculate the quantities η and ζ which are read in and are related in a simple manner -- see Eq. III.24. The quantities ϵ^a and ϵ^b are easily related to the cofactors generated by code 1. Code 1 will generate arbitrary cofactors depending upon input parameters.)

A more approximate method of calculating these quantities is provided directly in the two codes. Code 2 will obtain the solution for ϵ^r and B^S from a 4 level model (3 bound levels and 1 continuum level). Code 3 has the option of solving for ϵ^a and ϵ^b from a 3 level model (2 bound levels and 1 continuum level). These approximate solutions can be very useful for some purposes.

A symmetrical (about the center of the layer) geometrical grid (called Z in the program) is set up given the total geometric depth and number of desired decades. Currently, the maximum number of decades is set at 5 giving a total number of points of 31. This calls for solution

of a 31 x 31 matrix and may create underflow or overflow problems. The number of decades required for convergence must be tested for each problem.

Optical depth points at each geometric depth are next calculated from an integration over geometric depth at a given frequency.

Steps in frequency are now calculated using the quantities
 $x = \frac{v - v_o}{\Delta v_D}$ in the bound level cases and $y = v/v_{Kl}$ in the continuum. Step

sizes are input quantities and are constant in x and y . The maximum x is found by choosing the first value of x such that $e^{-x^2} \tau_{max} \leq 1.0$, and the maximum y such that $\tau_{max}/y^3 \leq 1.0$.

Certain quantities uniquely dependent on frequency are now calculated, such as $f(y)$, $g(y)$, $A(y)$, $f'(x)$, $g'(x)$, and $A'(x)$. A loop over frequency is set up with index k to compute the $W_{ijk}^{(\Lambda)}$ and $W_{ijk}^{(\Lambda-1)}$ (by means of the subroutine WMAT) and then sums over frequency are taken within the loop to arrive at the coefficients in the final equations: \bar{W}_{ij} in the bound case and M_{ij} in the continuum.

Once the integration over frequency is completed, the program sets up a matrix, called EM, for solution of the simultaneous equations to get S_j or $1/b_{ij}$. These are then punched in cards along with the population ratios to be used as inputs to the next step in the iteration.

The S_j or b_{ij} are used to determine new line or continuum radiative rates which are then used as input to code l. New values for the populations and the parameters ϵ_i^s , B_i^s , ϵ_i^a and ϵ_i^b are obtained and are used in beginning the next step of the iteration.

DESCRIPTION OF SUBPROGRAMS

SUBROUTINE WMAT (NZ, TCUT)

WMAT calculates $W_{ij}^{(1)}$ and $W_{ij}^{(N-1)}$ for those areas of the matrices where $|T_i - T_j|$ is less than TCUT.

FUNCTION NOSONI (A, X, L, LMAX)

NOSONI is a matrix inversion routine using the method outlined on page 434 of Hildebrand, Introduction to Numerical Analysis (New York, 1956).

A is a matrix of order L with column dimension LMAX. Its elements are assumed to be stored columnwise in the usual Fortran manner. X is working storage of length L. The inverse of A will replace A. Upon return, NOSONI = 1 if inversion went properly, = 0 if a divisor is zero, in which case, A may contain garbage.

FUNCTION ESB (X, N)

This routine uses the function EXIN to obtain $E_1(X)$, the exponential integral of order 1 in X. It then calculates $E_N(X)$, where $N = 2, 3$ or 4 from the recurrence relation $E_{N+1}(X) = \frac{1}{N} [e^{-X} - ZE_N(X)]$.

FUNCTION EXIN (Y)

EXIN obtains $E_1(Y)$ from polynomial approximations shown in sections 5.1.53 and 5.1.56 of the Handbook of Mathematical Functions, National Bureau of Standards, 1964.

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APPENDIX A
PROGRAM FOR SOLUTION OF STEADY STATE
EQUATIONS

95

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1*   C          P = 48A HELIUM
2*   C          SINGLE PRECISION
3*   C          VARIABLE R=ZERO
4*   C          ALL BETA AT TR
5* DIMENSION DA(2)
6* DIMENSION EV(3,19,19)
7* COMMON/BLK1/TAU(10),XJ(10,4),NTAU
8* 1/BLK2/OMEGA(3,19,19),AP(3,19,19),BB(3,19,19),OBAR(3,19,19),
9* 2DBAR(3,19,19),ABAR(3,19,19),Y(3,19,19),ALPH(3,19,19),BETA(3,19,19)
10* 3 /BLK3/XE,PI,H,CL,XK,XM,RCH,PAZ
11* 4/BLK4/E(3,19),EZ(3,19,19),F(3,19,19),G(3,19),ZB(3,19)
12* 5/BLK5/T,TR,N00,XNE,W,A(40,40),DIVIDE
13* 6/BLK6/LE,I1,I2,K7,K8,K9,IRO,ICO
14* 7/BLK7/EP8,E1,E2,AK(4),T1,S1BETA,S1C,S1AP,S1RZ
15* 8/BLK8/ZAN(40),XNEQ(40)
16* 9/BLK13/NL,NF,NT,MA(3),NST(3),MI(100),MJ(100),MK(100),NALPH
17* COMMON/BLK15/NFI(100),NFJ(100),NFK(100),NOF
18* CALL DATE(9,DA)
19* IZYX = 15
20* 10 DO 15 I=1,40
21*      DO 15 J=1,40
22* 15 A(I,J)=0,
23*      DO 20 I=1,3
24*      DO 20 J=1,19
25*      DO 20 K=1,19
26*      BETA(I,J,K)=0,
27*      EZ(I,J,K) = 0.0
28*      ABAR(I,J,K)=0.
29*      Y(I,J,K) = 0.0
30*      ALPH(I,J,K)=0,
31*      AP(I,J,K)=0.
32*      BB(I,J,K)=0.
33*      OBAR(I,J,K)=0.

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```

34*      DBAR(I,J,K)=0.
35*      OMEGA(I,J,K)=0.0
36*      20 F(I,J,K)=0.
37*      READ (5,40)NF,NT,NALPH,NOF
38*      NL = NF + NT + 1
39*      25 FORMAT(3I6,E12.8)
40*      DO 30 II=1,NOF
41*      READ (5,25)I,J,K,(F(I,J,K))
42*      MI(II) = I
43*      MJ(II) = J
44*      MK(II) = K
45*      NFI(II) = I
46*      NFJ(II) = J
47*      NFK(II) = K
48*      30 CONTINUE
49*      35 FORMAT(3I6,15X,2E15.8)
50*      40 FORMAT(12I6)
51*      45 FORMAT(6E12.8)
52*      READ (5,45)TR
53*      XLAM = 5.876E-05
54*      ANU = CL/XLAM
55*      IF (TR=1.0) 55,55,50
56*      50 EX = (H*ANU)/(XK*TR)
57*      DEN = EXP(EX) = 1.0
58*      BV = (2.0*H*ANU)**3/CL**2)/DEN
59*      GO TO 60
60*      55 BV = 0.0
61*      60 CONTINUE
62*      65 FORMAT(28H1ELECTRON TEMPERATURE (TE) =1PE11,4,10X,28HRADIATION 1
63*      1PERATURE (TR) =E11.4,10X,5HBNU =E11.4)
64*      DO 70 I=1,3
65*      DO 70 J=1,19
66*      DO 70 K=1,19
67*      IF (J.LE.K) GO TO 70
68*      F(I,K,J)=F(I,J,K)
69*      70 CONTINUE
70*      75 FORMAT(7H1HELIUM+10X,4HP48A,10X,8HPART ONE, 70X,A6,A3)
71*      WRITE (6,75)DA
72*      80 FORMAT(9HOF VALUES,22X,6HLAMBDA/)
73*      WRITE (6,80)
74*      85 FORMAT(3H F(I2,1H,I2,1H,I2,3H) =1PE10+3,E15.4)
75*      DO 90 II=1,NOF
76*      I = MI(II)
77*      J = MJ(II)
78*      K = MK(II)
79*      XL = 1.0E+08/ABS(E(I,J) - E(I,K))
80*      WRITE (6,85)I,J,K,F(I,J,K),XL
81*      90 CONTINUE
82*      DO 95 J=1,100
83*      MI(J) = 0
84*      MJ(J) = 0
85*      MK(J) = 0
86*      95 CONTINUE
87*      DO 100 II=1,NALPH
88*      READ (5,35)I,J,K,(ALPH(I,J,K)),BETA(I,J,K)
89*      MI(II) = I
90*      MJ(II) = J
91*      MK(II) = K

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```

92* 100 CONTINUE
93*   WRITE (6,65) T,TR,BV
94*   WRITE (6,105)
95* 105 FORMAT(1H0,22X,11HSTATISTICAL,15X,9HNUMBER OF,17X,19HENERGY VALUES
96*   ,1ABOVE/3X,3HION,3X,5HLEVEL,11X,6HWEIGHT,12X,21HOUTER SHELL ELECTRO
97*   2NS,9X,22HE(1:1) IN WAVE NUMBERS)
98*   DO 110 I=1,3
99*   NJ = NST(I)
100*   WRITE (6,115) I,(J,G(I,J),ZB(I,J),E(I,J),J=1,NJ)
101* 110 CONTINUE
102* 115 FORMAT(1H0,I4,I7,F17.0,F25.0,F34.2/(I12,F17.0,F25.0,F34.2))
103* 120 FORMAT(1H0,12X,3HI =,2X,1H2+19X+1H3//4X+1HK+8X+3HJ =,2X+1H1+19X+1H
104*   11/)
105* 125 FORMAT(1S+1P2E20.7)
106* 130 FORMAT(6H0I = 1)
107* 135 FORMAT(1H0,3X,1HJ+6X,3HK =,2X+1H1+17X+1H2+17X+1H3+17X,1H4+17X,1H5+
108*   117X+1H6+17X+1H7/)
109* 140 FORMAT(1H0,10X,3RK =,2X,1H8,17X+1H9,17X,2H10,16X,2H11,16X,2H12,16X
110*   1,2H13,16X,2H14/)
111* 145 FORMAT(1H0,3X,1HJ+6X,3HK =,2X+2H15,16X+2H16,16X+2H17,16X+2H18,16X+
112*   12H19/)
113* 150 FORMAT(6H0I = 2)
114* 155 FORMAT(1H0,3X,1HJ+8X,3HK =,2X+1H1+19X+1H2+19X+1H3+19X,1H4+19X+1H5,
115*   1/)
116* 160 FORMAT(1H0,12X,3HK =,2X+1H6+19X+1H7+19X+1H8+19X+1H9+19X+2H10)
117* 165 FORMAT(1S+1P7E18.7)
118* 170 FORMAT(1S+1P5E18.7)
119* 175 FORMAT(1S+1P5E20.7)
120* 180 FORMAT(13H1ALPHA(I,J,K),26X+25HRECOMBINATION COEFFICIENT)
121*   WRITE (6,180)
122*   WRITE (6,120)
123*   WRITE (6,125)(K,ALPH(2,1,K),ALPH(3,1,K),K=1,19)
124*   DO 185 I=1,3
125*   JL = NST(I)
126*   DO 185 J=1,JL
127*   DO 185 K=1,JL
128*   EZ(I,J,K) = ABS(E(I,J) - E(I,K))
129*   EV(I,J,K) = 1.23977E-04*EZ(I,J,K)
130* 185 CONTINUE
131*   WRITE (6,190)
132* 190 FORMAT(10H1DE(I,J,K),29X,36HENERGY DIFFERENCES IN ELECTRON VOLTS)
133*   WRITE (6,130)
134*   WRITE (6,135)
135*   WRITE (6,165)(J,(EV(1,J,K),K=1,7),J=1,19)
136*   WRITE (6,140)
137*   WRITE (6,165)(J,(EV(1,J,K),K=8,14),J=1,19)
138*   WRITE (6,190)
139*   WRITE (6,130)
140*   WRITE (6,145)
141*   WRITE (6,170)(J,(EV(1,J,K),K=15,19),J=1,19)
142*   WRITE (6,150)
143*   WRITE (6,155)
144*   WRITE (6,175)(J,(EV(2,J,K),K=1,5),J=1,10)
145*   WRITE (6,160)
146*   WRITE (6,175)(J,(EV(2,J,K),K=6,10),J=1,10)
147* C   CALCULATION OF CONSTANTS
148* CALL CONSTS
149* 195 CONTINUE

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150*      READ (5,45)T1,W,XNE
151*      READ (5,40)K7,K8,K9,LAST,LE,NTAU
152*      READ (5,45)(TAU(I),I=1,NTAU)
153*      READ (5,45)DIVIDE
154* 200  READ (5,40)NOY
155*      READ (5,40)IPROB,ILAST
156*      DO 205 I=1,3
157*      DO 205 J=1,19
158*      DO 205 K=1,19
159*      Y(I,J,K) = W
160* 205  CONTINUE
161*      NSWT = 0
162*      WRITE (6,210)
163* 210  FORMAT(1H1,53X,7H = 48A/54X,16HSINGLE PRECISION/54X,1SHVARIABLE
164*           1-ZERO/54X,27HGAUSS = HERMITE QUADRATURE)
165*      WRITE(6,215) T1,W,XNE,K7,K8,K9,LE,NTAU,DIVIDE,NSWT,(TAU(I),I=1,N
166*           1U)
167* 215  FORMAT(5H0T1 =1PE10,3/4H W =E10,3/6H XNE =E10,3/5H K7 =I3/5H K8
168*           13/5H K9 =I3/5H LE =I3/7H NTAU =I3/9H DIVIDE =E10,3/7H NSWT =I3/6
169*           2TAU =(E10,3))
170*      WRITE (6,220)NF,NT,NL
171* 220  FORMAT(5H NF =I2/5H NT =I2/5H NL =I2)
172*      WRITE (6,225)IPR0B
173*      FORMAT(15H1PROBLEM NUMBER,I4)
174*      IF (NOY) 230,260,230
175* 230  WRITE (6,235)
176*      FORMAT(9H0Y VALUES/)
177* 240  FORMAT(3H Y(I2,1H,I2,1H,I2,3H) =1PE9,2)
178*      DO 255 IJ=1,NOY
179*      READ (5,25)I,J,K,Y(I,J,K))
180*      XNU = CL*EZ(I,J,K)
181*      EY = (H*XNU)/(XK*T)
182*      EYZ = (H*XNU)/(XK*TR)
183*      IF ((EY,GT,.85,0)=OR,(EYZ,GT,.85,0)) GO TO 245
184*      B0 = 2.0*H*XNU*(XNU/CL**2)*XNU/(EXP(H*XNU/(XK*T)) = 1.0)
185*      BTR = 2.0*H*XNU*(XNU/CL**2)*XNU/(EXP(H*XNU/(XK*TR)) = 1.0)
186*      BOBTR = B0/BTR
187*      GO TO 250
188* 245  CONTINUE
189*      EXY = XNU*(H/XK)*(1.0/TR = 1.0/T)
190*      BOBTR = EXP(EXY)
191* 250  CONTINUE
192*      Y(I,J,K) = Y(I,J,K)*BOBTR
193*      Y(I,K,J) = Y(I,J,K)
194*      WRITE (6,240)I,J,K,Y(I,J,K)
195* 255  CONTINUE
196*      GO TO 275
197* 260  WRITE (6,265)
198* 265  FORMAT(17H0ALL Y(I,J,K) = W)
199*      WRITE (6,270)
200* 270  FORMAT(25H ALL ABAR MULTIPLIED BY W/37H ALL BB(I,J,K) MULTIPLIED
201*           (Y Y(I,J,K)/30H B(I,J,K) IN BB TABLE IS AT TR)
202* 275  WRITE (6,280)XNE,W
203* 280  FORMAT(5HINE =1PE11,4,10X,3HW =OPF7,2)
204*      WRITE (6,285)K7,K8,K9
205* 285  FORMAT(1H03X2HK7,4X2HK8,4X2HK9/3I6)
206*      CALL AMAT(0)
207*      HEM = 6.69E-24

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208* SQ = 2.0*XK*T/HEM
209* XNUM = SQRT(SQ)
210* DV = XNUM*ANU/CL
211* A94 = 7.06E+07
212* SIG = 3.74E+12/SQRT(T)
213* I7 = MA(K7)
214* DX = T1/(ZAN(I7)*SIG)
215* DI = ZAN(9)*A94*(H*ANU)/DV
216* DI = (DI*DX)/(4.0*PI*SQRT(PI))
217* WRITE (6,290)DI,DV,Dx
218* 290 FORMAT(9H0I/DELT =1PE11.4+10X,4HDV =E11.4+10X,4HDx =E11.4)
219* KK = 0
220* WRITE (6,295)IRO+ICO
221* 295 FORMAT(14H0ELIMINATE ROW,I3,5X,6HCOLUMN,I3)
222* XNU=CL*EZ(K7,K8,K9)
223* RHO = (XNU/CL)**2.0*H*XNU*G(K7,K9)/G(K7,K8)
224* EPS=OMEGA(K7,K8,K9)/AP(K7,K8,K9)*XNE
225* E1=E(K7,K8)
226* E2=E(K7,K9)
227* CALL ELIM(RHO,AP(K7,K8,K9))
228* DO 325 LY=1,NTAU
229* EY = (H*XNU)/(XK*T)
230* EYZ = (H*XNU)/(XK*TR)
231* IF ((EY,GT,85.0)*OR,(EYZ,GT,85.0)) GO TO 305
232* B0=2.*H*XNU*(XNU/CL**2)*XNU/(EXP(H*XNU/(XK*T))-1.)
233* BTR=2.*H*XNU*(XNU/CL**2)*XNU/(EXP(H*XNU/(XK*TR))-1.0)
234* B0BTR = B0/BTR
235* GO TO 310
236* 305 CONTINUE
237* EXY = XNU*(H/XK)*(1.0/TR - 1.0/T)
238* B0BTR = EXP(EXY)
239* 310 CONTINUE
240* FF = B0BTR
241* Y(K7,K8,K9) = FF
242* Y(K7,K9,K8) = FF
243* BBC=BBC(K7,K8,K9)*FF
244* BBD=BBD(K7,K9,K8)*FF
245* WRITE (6,315)TAU(LY),K7,K8,K9,BBC,K7,K9+K8,BBD+K7+K8+K9+K7,K9,K8,
246* 1F
247* 315 FORMAT(6H1TAU =1PE13.6,4X,5HBB*Y(I2,1H,I2,1H,I2,3H) =E13.6,4X,5H
248* 1*Y(I2+1H,I2+1H,I2+3H) =E13.6,4X,2HY(I2,1H+I2,1H,I2,4H), (I2+1H+I2
249* 21H,I2,3H) =E13.6)
250* WRITE (6,320)
251* 320 FORMAT(89X,13HY IS CONSTANT)
252* CALL AMAT(1)
253* DX = T1/(ZAN(I7)*SIG)
254* DI = ZAN(9)*A94*(H*ANU)/DV
255* DI = (DI*DX)/(4.0*PI*SQRT(PI))
256* WRITE (6,290)DI,DV,Dx
257* CALL ELIM(RHO,AP(K7,K8,K9))
258* 325 CONTINUE
259* 330 CONTINUE
260* GO TO (10,195,200),ILAST
261* END

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>DIAGNOSTICS

ITION TIME = 4.79 CPU SECONDS

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1* SUBROUTINE AMAT(KK)
2* DIMENSION CAP(40+40),RI(40),RJ(40),XN(5+19)
3* COMMON/BLK2/OMEGA(3,19+19),AP(3,19+19),BB(3,19+19),OBAR(3,19+19),
4* DBAR(3,19+19),ABAR(3,19+19),Y(3,19+19),ALPH(3,19,19),BETA(3,19+19)
5* 3 /BLK3/XE,PI,H,CL,XK,XM,RCH,PAZ
6* 4/BLK4/E(3,19),EZ(3,19,19),F(3,19,19),G(3,19),ZH(3,19)
7* 5/BLK5/T,TR,N00,XNE,W,A(40+40),DIVIDE
8* 5/BLK6/LE,I1,I2,K7,K8,K9,IRO,ICO
9* 7/BLK7/EPS,E1,E2,AK(4),T1,S1BETA+S1C,S1AP+S1RZ
10* 8/BLK8/ZAN(40),XNEQ(40)
11* 9/BLK13/NL,NF,NT,MA(3),NST(3),MI(100),MJ(100),MK(100),NALPH
12* COMMON/BLK15/NFI(100),NFJ(100),NFK(100),NOF
13* WRITE (6,10)KK
14* 10 FORMAT(17H1ENTER AMAT, KK =I2)
15* DO 115 I=NF,NL
16*   NSH = NST(I+1)
17*   NSL = NST(I-1)
18*   NS = NST(I)
19*   NSTART = MA(I)
20*   NEND = MA(I+1) - 1
21*   IF (I=3) 20+15,15
22*   15 NEND = NSTART
23*   20 K = 0
24*     DO 110 M=NSTART,NEND
25*       K = K + 1
26*       IF (I=NF) 35+35+25
27*       25 NJ = MA(I-1)
28*       NK = MA(I) - 1
29*       J = 0
30*       DO 30 N=NJ,NK
31*         J = J + 1
32*         A(M,N) = XNE*OBAR(I-1,J+K) + W*ABAR(I-1,J+K)
33*       30 CONTINUE
34*       35 J = 0
35*       DO 95 N=NSTART,NEND
36*         J = J + 1
37*         YY = Y(I,J,K)
38*         IF(KK,EQ,0) YY = W
39*         IF (M=N) 40+50+45
40*         40 A(M,N) = XNE*OMEGA(I,J,K) + YY*BB(I,J+K) + AP(I,J+K)
41*         GO TO 95
42*         45 A(M,N) = XNE*OMEGA(I,J,K) + BB(I,J+K)*YY
43*         GO TO 95

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44*      50 S0B = 0.0
45*      SAL = 0.0
46*      SOM = 0.0
47*      SAB = 0.0
48*      SRY = 0.0
49*      SDB = 0.0
50*      SAP = 0.0
51*      SBE = 0.0
52*      IF (I=NL) 55,65,65
53*      55 DO 60 L=1,NSH
54*      S0B = S0B + DBAR(I,J,L)
55*      SAB = SAB + ABAR(I,J,L)
56*      60 CONTINUE
57*      65 IF (I=NF) 80,80,70
58*      70 DO 75 LL=1,NSL
59*      SBE = SBE + BETA(I,J,LL)
60*      SDB = SDB + DBAR(I,J,LL)
61*      SAL = SAL + ALPH(I,J,LL)
62*      75 CONTINUE
63*      80 DO 90 L=1,NS
64*      IF (L.EQ.J) GO TO 85
65*      SOM = SOM + OMEGA(I,J,L)
66*      YY = Y(I,J,L)
67*      IF (KK.EQ.0) YY = W
68*      SBY = SBY + BB(I,J,L)*YY
69*      85 IF (L.GE.J) GO TO 90
70*      SAP = SAP + AP(I,J,L)
71*      90 CONTINUE
72*      A(M,N) = XNE*(S0B+SAL+SOM)-W*SAB-SBY-XNE*W*SRE-XNE*(XNE*SDB)-SAP
73*      95 CONTINUE
74*      IF (I=NL) 100,110,110
75*      100 NJ = MA(I+1)
76*      NK = NJ + NST(I+1) - 1
77*      J = 0
78*      DO 105 N=NJ,NK
79*      J = J + 1
80*      A(M,N) = XNE*(ALPH(I+1,J,K) + W*BETA(I+1,J,K) + XNE*DBAR(I+1,J,K))
81*      105 CONTINUE
82*      110 CONTINUE
83*      115 CONTINUE
84*      WRITE (6,120) DIVIDE
85*      120 FORMAT(18H0 DIVIDE MATRIX BY1PF12.4)
86*      IF (KK.NE.0) GO TO 130
87*      I1 = MA(NF)
88*      I2 = MA(NL) + NST(NL) - 1
89*      IRO=MA(K7)+K8-I1
90*      ICO = MA(K7) - I1 + 1
91*      NOO=I2-I1+1
92*      WRITE (6,125) LE,I1,I2,IRO,ICO,NOO
93*      125 FORMAT(1H0,3X,2HLE,4X,2HI1,4X,2HI2,3X,3HIRO,3X,3HIC0,3X,3HN00/6I6
94*      130 IF (I1.EQ.1) GO TO 140
95*      DO 135 I=1,NOO
96*      DO 135 J=1,NOO
97*      IL=I1-1+I
98*      IM=I1-1+J
99*      A(I,J)=A(IL,IM)
100*     135 A(IL,IM)=0,
101*     140 DO 145 I=1,NOO

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102*      DO 145 J=1,N00
103*      145 A(I,J) = A(I,J)/DIVIDE
104*      WRITE (6,150)
105*      150 FORMAT(65H0Q(I) = SUM OF ALL ELEMENTS IN COLUMN I OF RATE EQUATI
106*      (ON MATRIX/)
107*      DO 165 I=1,N00
108*      QT=0.
109*      DO 155 J=1,N00
110*      155 QT=QT+A(J,I)
111*      WRITE (6,160) I,QT
112*      160 FORMAT(3H Q(I2,3H) =,PE15.6)
113*      165 CONTINUE
114*      IF (KK) 170,170,175
115*      170 WRITE (6,300)
116*      GO TO 180
117*      175 WRITE (6,305)
118*      180 DO 185 I=1,N00
119*      185 WRITE (6,190) I,(A(I,J),J=1,N00)
120*      190 FORMAT(1H0,I3,2X,1P9E14.4/(6X,9E14.4))
121*      WRITE (6,320)
122*      DO 200 LC=1,N00
123*      DO 200 LR=1,N00
124*      IF (LC.GT.2,AND.LR.GT.2) GO TO 200
125*      CAP(LR,LC)=COFACT(LR,LC,N00,A)
126*      WRITE (6,195) LR,LC,CAP(LR,LC)
127*      195 FORMAT(22H COFACTOR OF ELEMENT A,2I4,2X,1H=1PE15.6)
128*      200 CONTINUE
129*      PP=0.
130*      DO 205 I=1,N00
131*      205 PP=PP+CAP(1,I)
132*      ALAMB=1./PP
133*      ASUM=0.
134*      CF1=2./XNE*(SQRT(2.*PI*(XM/H)*T)*SQRT(XK/H))**3
135*      JF = 0
136*      DO 215 J=NF,NL
137*      JL = NST(J)
138*      DO 210 I=1,JL
139*      JF = JF + 1
140*      PPO = (E(J,I) - E(LE,1))*H*CL/(XK*T)
141*      P2 = 0.5*PPO
142*      EX = EXP(-P2)
143*      RI(JF) = CF1**((J-LE)*G(J,I)/G(LE,1)*EX
144*      RI(JF) = RI(JF)*EX
145*      ASUM = ASUM + RI(JF)
146*      210 CONTINUE
147*      215 CONTINUE
148*      DO 220 I=1,N00
149*      ZAN(I) = ALAMB*CAP(1,I)
150*      220 CONTINUE
151*      WRITE (6,225) ALAMB,ASUM
152*      225 FORMAT(10H0ALAMBDA1 =1PE15.6,5X,9HLAMBDAE =,E15.6)
153*      IF (KK) 230,230,235
154*      230 WRITE (6,310)
155*      GO TO 240
156*      235 WRITE (6,315)
157*      240 DO 250 I=1,N00
158*      LX=I1+I-1
159*      XNEQ(I) = RI(I)/ASUM

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160*      RJ(I) = ZAN(I)/XNEQ(I)
161*      WRITE (6,245)LX,ZAN(T),RJ(I),XNEQ(I)
162*      245 FORMAT(13+2X+3HN =,1PE15.7+2X+7HN/NEQ =,E15.7+2X+5HNEQ =,E15.7)
163*      250 CONTINUE
164*      GO TO (255,260),K7
165*      255 SIG23 = 3.74E-12/SQRT(T)
166*      XN20 = ZAN(1)*XNE/10.0
167*      GO TO 265
168*      260 SIG23 = 2.84E-12/SQRT(T)
169*      XN20 = ZAN(20)*XNE/10.0
170*      265 HH = T1/(XN20*SIG23)
171*      WRITE (6,270)HH
172*      270 FORMAT(4H0H =1PE11.4)
173*      IJ = 0
174*      DO 280 I=NF,NL
175*      JL = NST(I)
176*      DO 275 J=1,JL
177*      IJ = IJ + 1
178*      XN(I,J) = ZAN(IJ)
179*      275 CONTINUE
180*      280 CONTINUE
181*      WRITE (6,285)
182*      285 FORMAT(11H1( I, J, K),5X,1HF,11X,2HOD)
183*      DO 295 L=1,NUF
184*      I = NFI(L)
185*      J = NFJ(L)
186*      K = NFK(L)
187*      OD = (XN(I,K)/XN(K7,K9))*(F(I,K,J)/F(K7,K9,K8))*(EZ(K7,K9,K8)/
188*      ;EZ(I,K,J))*T1
189*      WRITE (6,290)I,K,J,F(I,K,J),OD
190*      290 FORMAT(2H (I2,1H,I2,1H,I2,1H)+1PE10.3+E15.7)
191*      295 CONTINUE
192*      RETURN
193*      300 FORMAT(1H1,2X,1HI,50X,20HRATE EQUATION MATRIX)
194*      305 FORMAT(1H1,2X,1HI,35X,52HRATE EQUATION MATRIX INCLUDING THICK RAD]
195*      IATION FIELD)
196*      310 FORMAT(24H1OPTICALLY THIN SOLUTION/)
197*      315 FORMAT(44H1SOLUTION INCORPORATING THICK RADIATION FIELD/)
198*      320 FORMAT(1H1)
199*      END

```

DIAGNOSTICS

UTION TIME = 3.87 CPU SECONDS

```

1* BLOCK DATA
2* COMMON/BLK3/XE,PI,H,CL,XK,XM,RCH,PAZ
3* 4/BLK4/E(3,19),EZ(3,19,19),F(3,19,19),G(3,19),ZR(3,19)
4* 9/BLK13/NL,NF,NT,MA(3),NST(3),MI(100),MJ(100),MK(100),NALPH
5* DATA MA/1,20,30/NST/19,10,1/
6* DATA ((G(I,J),J=1,19),I=1,3)/1,3,1,9,3,3,1,9,15,5,3,3,
7* 11,9,15,5,27,7,3,
8* 22,2,6,2,6,10,2,6,10,14,9*0,
9* 31,18*0,/
10* DATA ((E(I,J),J=1,19),I=1,3)/0,,159850.32,166271.70,169081.50,
11* 1171129.15,183231.08,184859.06,185559.09,186095.90,186099.22,
12* 1186203.62,190292.46,190934.50,191211.42,191438.83,191440.71,
13* 191446.61,191447.24,191486.95,
14* 2198305.00,527484.57,527487.02,588445.76,588446.49,588447.64,
15* 2609781.98,609782.28,609782.77,609782.95,9*0.0,
16* 3637213.67,18*0.0/
17* DATA ((ZR(I,J),J=1,19),I=1,2)/19*2,,10*1,,9*0,/
18* DATA XE,PI,H,CL,XK,XM,RCH,PAZ/4,803E-10,3,1416,6,6256E-27,
19* 1,2.9979E10+1.3805E-16,9,1091E-28,2,179E-11+8,797E-17/
20* END

```

GNOSTICS

ON TIME = .52 CPU SECONDS

```

1* FUNCTION COFACT(NR,NC,NE,D)
2* DIMENSION D(40,40),E(40,40)
3* MN = 40
4* NP=NE=1
5* DO 10 I=1,NP
6* IR=I
7* IF(I.GE.NR) IR=I+1
8* DO 10 J=1,NP
9* IC=J
10* IF(J.GE.NC) IC=J+1
11* 10 E(I,J)=D(IR,IC)
12* Y = 1.0
13* M = NDETRM(MN,NP,E,Y)
14* IF (M=2) 30,15,20
15* 15 WRITE (6,35)NR,NC,Y
16* GO TO 25
17* 20 WRITE (6,40)NR,NC
18* 25 Y = 0.0
19* 30 LT = NR + NC
20* MZ=MOD(LT,2)
21* Z=1.
22* IF(MZ,NE,0) Z=1.
23* COFACT=Z*Y
24* RETURN
25* 35 FORMAT(23H0***** OVER/UNDERFLOW+10X,4HN R =13,10X,4HN C =13,1
26* 1Y =1PE11.4)
27* 40 FORMAT(24H0***** SINGULAR MATRIX,10X,4HN R =13,10X,4HN C =13)
28* END

```

```

1* FUNCTION COLL(T,I,J,K,N)
2* DIMENSION EV(3,19,19),A(3,19,19),AN(3,19,19),AL(3,19,19),AB(2),
3* ABN(2),ABL(2)
4* COMMON/BLK3/XE,P1,H,CL,XK,XM,RCH,PAZ
5* COMMON/BLK4/E(3,19),EZ(3,19,19),F(3,19,19),G(3,19),ZB(3,19)
6* DATA (A(1+1,L),L=2,19)/1.52E=10,6.68E=11,1.38E=10+6,01E=15,
7* 15.03E=16,1.08E=17,3.20E=11,8.11E=13,6.24E=18,2.36E=15,1.14E=15,
8* P1.18E=17,5.25E=12,2.25E=13,1.87E=21,3.01E=15,1.36E=18,4.88E=16/
9* DATA (A(1+2,L),L=3,19)/1.10E=06,9.47E=09,4.56E=08+4.34E=09,
10* 16.03E=09,5.38E=09,8.36E=09,7.72E=07,4.06E=07,7.27E=10,1.08E=09,
11* 23.99E=10,1.21E=09,8.44E=08,2.46E=10,1.48E=08,3.75E=08/
12* DATA (A(1+3,L),L=4,5)/4.45E=07,1.00E=07/
13* DATA (AN(1+1,L),L=2,19)/0.427+0.498+0.476+1.39+1.41+1.68+0.489+
14* 10.520+1.72+1.36+1.24,1.61+0.594,0.580+2.32+0.555,1.27+1.39/
15* DATA (AN(1+2,L),L=3,19)/-0.196,0.586,0.154,0.390,0.348,0.287,
16* 10.394,-0.164,-0.135+0.413,0.230+0.410+0.441,-0.0514,0.423,
17* 2+0.0663,-0.024/
18* DATA (AN(1+3,L),L=4+5)/-0.0617+0.389/
19* DATA (AL(1+1,L),L=2,19)/0.999+1.0+1.01+1.0,1.01+0.995,1.01,1.02,
20* 10.997,1.0+1.01,0.997,1.01+1.02,0.976,1.02+1.01+1.0/
21* DATA (AL(1+2,L),L=3,19)/1.41+1.36+1.28+1.15,3+1.12,2*1.18+1.07,
22* 11.14+1.05+1.12,1.09+1.13+1.09+1.10/
23* DATA (AL(1+3,L),L=4+5)/1.43+1.72/
24* DATA (AB(L),L=1,2)/6.99E=15+1.02E=14/
25* DATA (ABN(L),L=1,2)/1.44+1.23/
26* DATA (ABL(L),L=1,2)/1.0+1.01/
27* XKT = XK*T/1.602E=12
28* EV(I,J,K) = 1.23977E=04*EZ(I,J,K)
29* GO TO (10+15),N
30* 10 EX = AL(I,J,K)*EV(I,J,K)/XKT
31* A1 = T**AN(I,J,K)
32* A2 = EXP(-EX)
33* COLL = A(I,J,K)*A1*A2
34* RETURN
35* 15 EF = ABS(E(I+1,K) - E(I,J))
36* EG = 1.23977E=04*EF
37* EX = ABL(I)*EG/XKT
38* A1 = T**ABN(I)
39* A2 = EXP(-EX)
40* COLL = AB(I)*A1*A2
41* RETURN
42* END

```

IAGNOSTICS

TION TIME = .90 CPU SECONDS

```

1*      SUBROUTINE CONSTS
2*      COMMON /BLK3/XE,PI,H,CL,XK,XM,RCH,PAZ
3*      3/BLK2/OMEGA(3,19,19),AP(3,19,19),BB(3,19,19),OBAR(3,19,19),
4*      4DBAR(3,19,19),ABAR(3,19,19),Y(3,19,19),ALPH(3,19,19),BETA(3,19,19)
5*      4/BLK4/E(3,19),EZ(3,19,19),F(3,19,19),G(3,19),ZB(3,19)
6*      5/BLKS/T,TR,N00,XNE,W,A(40,40),DIVIDE
7*      9/BLK13/NL,NF,NT,MA(3),NST(3),MI(100),MJ(100),MK(100),NALPH
8*      DATA B,AX,D,DP,EP,ADP,DDP/-0.0625+0.9321+0.0625+0.004,17+-0.15+0.025/
9*      10 FORMAT(1H0,12X,3H1 =,2X+1H2+19X+1H3//4X+1HK+8X+3HJ =,2X+1H1+19X+1H
10*           11)
11*      15 FORMAT(I5+1P2E20.7)
12*      20 FORMAT(1H0,12X,3H1 =,2X+1H1+19X+1H2//4X+1HJ+8X+3HK =,2X+1H1+19X+1H
13*           11)
14*      25 FORMAT(6H0I = 1)
15*      30 FORMAT(1H0,3X+1HJ+6X,3HK =,2X+1H1+17X+1H2+17X+1H3+17X,1H4+17X,1H5+
16*           117X+1H6+17X,1H7/)
17*      35 FORMAT(1H0,10X,3HK =,2X+1H8+17X+1H9,17X+2H10,16X,2H11,16X+2H12+16X+
18*           1+2H13+16X+2H14/)
19*      40 FORMAT(1H0,3X+1HJ+6X,3HK =,2X+2H15+16X+2H16+16X+2H17+16X+2H18+16X+
20*           12H19/)
21*      45 FORMAT(6H0I = 2)
22*      50 FORMAT(1H0,3X+1HJ+8X,3HK =,2X+1H1+19X+1H2+19X+1H3+9X+1H4+19X+1H5+
23*           11)
24*      55 FORMAT(1H0,12X,3HK =,2X+1H6+19X+1H7,19X+1H8+19X+1H9+19X+2H10/)
25*      60 FORMAT(I5+1P7E18.7)
26*      65 FORMAT(I5+1P5E18.7)
27*      70 FORMAT(I5+1P5E20.7)
28*      TE = T
29*      TRTE = TR/TE
30*      FF1 = (SQRT(2.*PI*(XM/H)*TE)*SQRT(XK/H))**3
31*      FF2 = FF1*TRTE**1.5
32*      HCKT=H*CL/(XK*TE)
33*      HCKTR = HCKT/TRTE
34*      TAB = ABS(TRTE - 1.0)
35*      T1=SQRT(TE)
36*      FFF=1./FF1
37*
38*      C      **** ORIGINALLY SUOBA ****
39*      DO 130 IJ=1,NALPH
40*      IF (TAB,LT,1.0E-05) GO TO 80
41*      READ (5,75)I,K,J,TTR,AL,BE
42*      75 FORMAT(3I6,3E15.8)
43*      BETA(I,K,J) = BE

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```

44* GO TO 85
45* 80 I = MI(IJ)
46* K = MJ(IJ)
47* J = MK(IJ)
48* TTR = TR
49* AL = ALPH(I,K,J)
50* BE = BETA(I,K,J)
51* 85 I = I + 1
52* EF=ABS(E(I+1,K)-E(I,J))
53* X = I
54* EZ2=EF*CL*H/1.6021E-12
55* XZ=EF*HCKT
56* FF3 = AL + BE
57* ARG = EF*HCKTR
58* IF (ARG.GE.88.0) GO TO 90
59* Y2 = EXP(-ARG)
60* GO TO 95
61* 90 Y2 = 0.0
62* 95 ABAR(I,J,K) = 2.0*G(I+1,K)/G(I,J)*Y2*FF2*FF3
63* IF (XZ.GE.88.) GO TO 100
64* Y1=EXP (-XZ)
65* GO TO 105
66* 100 Y1=0.
67* 105 F1 = (3.1 - 1.2/X - .9/X**2)
68* IF ((J.EQ.1).AND.(K.EQ.1)) GO TO 110
69* OBAR(I,J,K)=1.15E-8*F1*ZB(I,J)*T1*Y1/EZ2**2
70* GO TO 115
71* 110 OBAR(I,J,K) = COLL(T,I,J,K,2)
72* 115 CONTINUE
73* IF (XZ.GE.88.) GO TO 120
74* DBAR(I+1,K,J)=G(I,J)/G(I+1,K)/2.*EXP(XZ)*FFF*OBAR(J,J,K)
75* GO TO 125
76* 120 DBAR(I+1,K,J)=0.0
77* 125 CONTINUE
78* 130 CONTINUE
79* WRITE (6,135)
80* 135 FORMAT(12H1BETA(I,J,K),27X,42HSTIMULATED RECOMBINATION COEFFICIENT
81* ,1 AT TR)
82* WRITE (6,140)
83* 140 FORMAT(1H0,12X,3H1 =,2X+1H2+19X+1H3//4X,1HK+8X,3HJ =,2X+1H1+19X+1H
84* 11/)
85* WRITE (6,145)(K,BETA(2+1,K)+BETA(3+1,K),K=1,19)
86* 145 FORMAT(15+1P2E20.7)
87* WRITE (6,150)
88* 150 FORMAT(12H1DBAR(I,J,K),27X,43HELECTRON COLLISIONAL IONIZATION COEF
89* FICIENT)
90* WRITE (6,20)
91* WRITE (6,15)(J,DBAR(1,J+1)+DBAR(2+J,1),J=1,19)
92* WRITE (6,155)
93* 155 FORMAT(12H1DBAR(I,J,K),27X,46HELECTRON COLLISIONAL RECOMBINATION CO
94* EFFICIENT)
95* WRITE (6,10)
96* WRITE (6,15)(K,DBAR(2+1,K)+DBAR(3+1,K),K=1,19)
97* C
98* WRITE (6,160)TTR
99* 160 FORMAT(12H1ABAR(I,J,K),24X,33HRADIATIVE IONIZATION RATE AT TR =1PE
100* 111.4)
101* WRITE (6,20)

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102*      WRITE (6,15)(J,ABAR(j,j+1),ABAR(2+j,1),j=1,19)
103*      C
104*      C **** ORIGINALLY COMBB ****
105*      XK2 = XK*SQRT(XK)
106*      T2 = T*SQRT(T)
107*      C38=32.*PI/SQRT(3.)*PAZ/SQRT(2.*PI*XH)*RCH**2/XK2
108*      C39=4.*RCH*PAZ/(SQRT(XH*TE)*SQRT(2.*PI*XK))
109*      WRITE (6,165)
110* 165 FORMAT(1H1,3X,1H1,4X,1HJ,4X,1HK,1IX,BHB(I,J,K),12X,BHB(I,K,J)/)
111*      DO 280 I=1,3
112*      JL = NST(I)
113*      DO 280 J=1,JL
114*      DO 280 K=1,JL
115*      EV = 1.23977E-04*EZ(I,J,K)
116*      ENZ = EV/13.6
117*      XZ=EZ(I,J,K)*HCKT
118*      EX1 = EXP(-XZ)
119*      EX2 = EX1**2
120*      EX10 = EX1**10
121*      EX17 = EX1**17
122*      EX30 = EX1**30
123*      EX100 = EX10**10
124*      IF (XZ,GE,88.0) GO TO 170
125*      Y1=EXP(-XZ)
126*      GO TO 175
127* 170 Y1=0.0
128* 175 IF (J,GE,K) GO TO 280
129*      IF (I,GT,1) GO TO 215
130*      IF (J,EQ,1) GO TO 245
131*      IF (J,EQ,2) GO TO 245
132*      IF ((J,EQ,3).AND.(K,EQ,4)) GO TO 245
133*      IF ((J,EQ,3).AND.(K,EQ,5)) GO TO 245
134*      IF (F(I,K,J),LE,1.0E-7) GO TO 190
135*      C
136*      C **** ORIGINALLY SU36 ****
137*      Y2=Y1/XZ
138*      Z=1./XZ
139*      IF (EP*XZ,GE,88.0) GO TO 180
140*      Y3=EXP(-XZ*EP)/XZ
141*      GO TO 185
142* 180 Y3=0.0
143* 185 F1 = 0.14*EX1
144*      F2 = -0.083*EX2
145*      F3 = -0.053*EX17
146*      OMEGA(I,J,K) = C38*F(I,J,K)*(F1 + F2 + F3)/(T2*XZ**2)
147*      GO TO 250
148*      C
149*      C **** ORIGINALLY SU37 ****
150* 190 C=C39/G(I,J)
151*      YD=RCH/(XK*TE)
152*      XZ1=XZ+YD
153*      IF (XZ1,GE,88.) GO TO 195
154*      F3=EXP(-XZ1)
155*      F1=F3*(1.+YD)
156*      GO TO 200
157* 195 F1=0.0
158*      F3=0.0
159* 200 IF (XZ,GE,88.) GO TO 205

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```

60*      F2=EXP(-XZ)
61*      GO TO 210
62*      205 F2=0.0
63*      210 OMEGA(I,J,K)=C*((F2=F1)/Y0+F3)
64*      OMEGA(I,J,K) = OMEGA(I,J,K)/ENZ
65*      GO TO 250
66*      215 IF (F(I,K,J).LE.1.E-7) GO TO 240
67*
68*      C      M***** ORIGINALLY SU38 ****
69*      Y2=Y1/XZ
70*      IF (2.*XZ.GE.88.0) GO TO 220
71*      Y3=EXP(-2.*XZ)/XZ
72*      GO TO 225
73*      220 Y3=0.0
74*      225 IF (48.*XZ.GE.88.) GO TO 230
75*      Y4=EXP(-48.*XZ)/XZ
76*      GO TO 235
77*      230 Y4=0.0
78*      235 F1 = 0.2*EX1
79*      F2 = (0.045/XZ)*EX2
80*      F3 = -(0.024/XZ)*EX10
81*      F4 = -(0.016/XZ)*EX30
82*      F5 = -(1.33 + 0.005/XZ)*EX100
83*      OMEGA(I,J,K) = C38*F(I,J,K)*(F1 + F2 + F3 + F4 + F5)/(T2*XZ)
84*      GO TO 250
85*
86*      C      **** ORIGINALLY SU39 ****
87*      240 OMEGA(I,J,K)=C39*Y1/G(I,J)
88*      OMEGA(I,J,K) = OMEGA(I,J,K)/ENZ
89*      GO TO 250
90*      245 OMEGA(I,J,K) = COLL(T,I,J,K+1)
91*      250 IF (XZ.GE.88.) GO TO 255
92*      OMEGA(I,K,J)=G(I,J)/G(I,K)*EXP(XZ)*OMEGA(I,J,K)
93*      GO TO 260
94*      255 OMEGA(I,K,J)=0.0
95*      260 IF (F(I,K,J).LE.1.E-7) GO TO 280
96*      XNU=CL*EZ(I,K,J)
97*      CAP=8.*PI**2*(XE**2/XM)*(XNU/CL)**2*(XNU/CL)
98*      AP(I,K,J)=G(I,J)/G(I,K)*CAP*F(I,K,J)
99*      BVIJK = 4.0*PI**2*XE**2*F(I,K,J)/((XM*CL)*(H*XNU))
200*      BVIKJ = G(I,J)/G(I,K)*BVIJK
201*      WRITE (6,265) I,J,K,BVIJK,BVIKJ
202*      265 FORMAT(3I5,1P2E20.4)
203*      ARG = H*XNU/(XK*TR)
204*      ARG = 0.5*ARG
205*      IF (ARG=88.0) 275,270,270
206*      270 BB(I,J,K) = 0.0
207*      BB(I,K,J) = 0.0
208*      GO TO 280
209*      275 PART = EXP(ARG)
210*      PLFT = (2.0*H*XNU)*(XNU/CL)**2/(PART - 1.0)
211*      BB(I,J,K) = (PLFT*BVIJK)/(PART + 1.0)
212*      BB(I,K,J) = (PLFT*BVIKJ)/(PART + 1.0)
213*      280 CONTINUE
214*      WRITE (6,285)
215*      285 FORMAT(13H10MEGA(I,J,K),26X,43HELECTRON COLLISIONAL EXCITATION COE
216*      IFFICIENT)
217*      WRITE (6,25)

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218*      WRITE (6,30)
219*      WRITE (6,60)(J,(OMEGA(1+J,K),K=1,7),J=1,19)
220*      WRITE (6,35)
221*      WRITE (6,60)(J,(UMEGA(1+J,K),K=8,14),J=1,19)
222*      WRITE (6,285)
223*      WRITE (6,25)
224*      WRITE (6,40)
225*      WRITE (6,65)(J,(OMEGA(1+J,K),K=15,19),J=1,19)
226*      WRITE (6,45)
227*      WRITE (6,50)
228*      WRITE (6,70)(J,(OMEGA(2+J,K),K=1,5),J=1,10)
229*      WRITE (6,55)
230*      WRITE (6,70)(J,(UMEGA(2+J,K),K=6,10),J=1,10)
231*      WRITE (6,290)
232* 290 FORMAT(10H1AP(I,J,K),29X,43HEINSTEIN SPONTANEOUS TRANSITION PROBAB
233*    ILITY)
234*      WRITE (6,25)
235*      WRITE (6,30)
236*      WRITE (6,60)(J,(AP(1,J,K),K=1,7),J=1,19)
237*      WRITE (6,35)
238*      WRITE (6,60)(J,(AP(1,J,K),K=8,14),J=1,19)
239*      WRITE (6,290)
240*      WRITE (6,25)
241*      WRITE (6,40)
242*      WRITE (6,65)(J,(AP(1,J,K),K=15,19),J=1,19)
243*      WRITE (6,45)
244*      WRITE (6,50)
245*      WRITE (6,70)(J,(AP(2,J,K),K=1,5),J=1,10)
246*      WRITE (6,55)
247*      WRITE (6,70)(J,(AP(2,J,K),K=6,10),J=1,10)
248*      WRITE (6,295)
249* 295 FORMAT(10H1BB(I,J,K),29X,42HEINSTEIN ABSORPTION TRANSITION PROBAB
250*    ILITY)
251*      WRITE (6,25)
252*      WRITE (6,30)
253*      WRITE (6,60)(J,(BB(1,J,K),K=1,7),J=1,19)
254*      WRITE (6,35)
255*      WRITE (6,60)(J,(BB(1,J,K),K=8,14),J=1,19)
256*      WRITE (6,295)
257*      WRITE (6,25)
258*      WRITE (6,40)
259*      WRITE (6,65)(J,(BB(1,J,K),K=15,19),J=1,19)
260*      WRITE (6,45)
261*      WRITE (6,50)
262*      WRITE (6,70)(J,(BB(2,J,K),K=1,5),J=1,10)
263*      WRITE (6,55)
264*      WRITE (6,70)(J,(BB(2,J,K),K=6,10),J=1,10)
265*      RETURN
266*      END

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>DIAGNOSTICS

ITION TIME = 4.97 CPU SECONDS

```
1*      SUBROUTINE ELIM(RHO,AP)
2* C*****THIS SUBROUTINE COMPUTES DOUBLE COFACTORS AND USES THEM
3* C*****TO COMPUTE ETA AND IOTA
4* COMMON/BLK5/T,TR,N00,XNE,W,A(40,40),DIVIDE
5* 1/BLK6/LE,I1,I2,K7,K8,K9,IRO,ICO
6* 2/BLK7/ EPS,E1,E2,XK( 4 ),T1,BETA,C,AQ,RZ
7* DIMENSION RMAT(40,40),ID(4)
8* DATA ID/1HU,1HV,2HS4,2HS5/
9* MN = 40
10* N002 = N00 = 2
11* S=0.
12* S1=0.
13* WRITE (6,10)
14* 10 FORMAT(54H0DOUBLE COFACTORS USED TO COMPUTE ETA AND IOTA IN ELIM/6
15* 11H SIGN FOR DEFINITION OF COFACTOR IS (-1)**(R1 + R2 + C1 + C2)/48
16* 2H THIS SIGN CHANGES WHENEVER R2 > R1 OR C2 > C1//,10H ELIMINATE,2
17* 3X,11HR1 C1 R2 C2,21X,11HR1 C1 R2 C2)
```

```

18*      DO 60 KM=1,N00
19*      IF ((KM,EQ,IRO),OR,(KM,EQ,ICO)) GO TO 60
20*      C*****SUBROUTINE ELM2 ELIMINATES 2 ROWS AND 2 COLUMNS
21*      C*****FROM ORIGINAL MATRIX AND PLACES THE N=2 MATRIX INTO
22*      C*****RMAT AND THEN THE DOUBLE COFACTOR IS COMPUTED
23*      CALL ELM2(IRO,ICO,KM,IRO,RMAT,Z)
24*      U = 1.0
25*      M = NDETRM(MN,N002,RMAT+U)
26*      IF (M=2) 30,15,20
27*      15 WRITE (6,115) IRO,ICO,ID(1)
28*      GO TO 25
29*      20 WRITE (6,120) IRO,ICO,ID(1)
30*      25 U = 0.0
31*      30 U = U*Z
32*      CALL ELM2(ICO,IRO,KM,ICO,RMAT,Z)
33*      V = 1.0
34*      M = NDETRM(MN,N002,RMAT+V)
35*      IF (M=2) 50,35,40
36*      35 WRITE (6,115) IRO,ICO,ID(2)
37*      GO TO 45
38*      40 WRITE (6,120) IRO,ICO,ID(2)
39*      45 V = 0.0
40*      50 V = V*Z
41*      IF(KM,GT,IRO) U = -U
42*      IF(IRO,GT,ICO) U = -U
43*      IF(KM,GT,ICO) V = -V
44*      IF(ICO,GT,IRO) V = -V
45*      C*****A IS THE MATRIX ELEMENT, U AND V ARE THE DOUBLE COFACTORS
46*      C*****THE MATRIX WAS DIVIDED BY DIVIDE TO PREVENT OVERFLOW WHEN
47*      C*****THE COFACTORS ARE BEING COMPUTED. THIS MUST BE TAKEN INTO
48*      C*****ACCOUNT HERE
49*      S=S+A(KM,IRO)*U*DIVIDE
50*      S1=S1+A(KM,ICO)*V*DIVIDE
51*      WRITE (6,55) IRO,ICO,KM,IRO,U,ICO,IRO,KM,ICO+V
52*      55 FORMAT(10X,4I3,2X,1PE15.6,5X,4I3,2X,E15.6)
53*      60 CONTINUE
54*      CALL ELM2(IRO,ICU,ICO,IRO,RMAT,Z)
55*      S4 = 1.0
56*      M = NDETRM(MN,N002,RMAT+S4)
57*      IF (M=2) 80,65,70
58*      65 WRITE (6,115) IRO,ICO,ID(3)
59*      GO TO 75
60*      70 WRITE (6,120) IRO,ICO,ID(3)
61*      75 S4 = 0.0
62*      80 S4 = S4*Z
63*      S4 = -S4
64*      WRITE (6,105) IRO,ICO,ICO,IRO,S4
65*      CALL ELM2(ICO,IR0,IRO,ICO,RMAT,Z)
66*      S5 = 1.0
67*      M = NDETRM(MN,N002,RMAT+S5)
68*      IF (M=2) 100,85,90
69*      85 WRITE (6,115) IRO,ICO,ID(4)
70*      GO TO 95
71*      90 WRITE (6,120) IRO,ICO,ID(4)
72*      95 S5 = 0.0
73*      100 S5 = S5*Z
74*      S5 = -S5
75*      WRITE (6,105) ICO,IRO,IRO,ICO,S5

```

```

6* 105 FORMAT(10X,4I3,2X,1PE15.6)
7*   ETA=1./S4*S/AP
8*   XIOTA=RHO/S4*S1/AP
9*   WRITE(6,110) ETA,XIOTA,EPS
0* 110 FORMAT(1H0,5HETA =1PE15.6,10X,6HIOTA =E15.6,10X,5HEPS =E15.6)
1*   WRITE(6,111) S,S1
2* 111 FORMAT(4H S =1pE14.7,10X,4HS1 =E14.7)
3*   WRITE(6,11) T1,T2,W,E1,E2,TR
4* 11 FORMAT(7X,2H†1,14X,2HTE+14X,1HW,15X,2HE1+14X,2HE2+14X,2HTR/(1P6E16
5*   1.6))
6*   RETURN
7* 115 FORMAT(21H0*****UNDER/OVERFLOW,10X,5HROW =I3,10X,5HCOL =I3+10X,A6
8*   1)
9* 120 FORMAT(22H0*****SINGULAR MATRIX,10X,5HROW =I3+10X,5HCOL =I3+10X,A
9*   16)
91*   END

```

AGNOSTICS

ION TIME = 1.46 CPU SECONDS

```
1*      SUBROUTINE ELM2(IRA,ICA,KRA,KCA,RMAT,Z)
2*      COMMON/BLKS/T,TR,N00,XNE,W,A(40,40),DIVIDE
3*      DIMENSION RMAT(40,40)
4*      IRO=IRA
5*      ICO=ICA
6*      KRO=KRA
7*      KC0=KCA
8*      IF (IRO.LE.KRO) GO TO 10
9*      ISR=IRO
10*     ISC=KRO
11*     IRO=ISC
12*     KRO=ISR
13*     10 IF (ICO.LE.KC0) GO TO 15
14*     ISR=ICO
15*     ISC=KC0
16*     IC0=ISC
17*     KC0=ISR
18*     15 NN=N00-2
19*     DO 45 IJK=1,NN
20*     IF (IJK.GE.IRO) GO TO 20
21*     NP=IJK
22*     GO TO 30
23*     20 IF (IJK.GE.KRO-1) GO TO 25
24*     NP=IJK+1
25*     GO TO 30
26*     25 NP=IJK+2
27*     30 DO 45 KO=1,NN
28*     IF (KO.GE.IC0) GO TO 35
29*     NR=KO
30*     GO TO 45
31*     35 IF (KO.GE.KC0-1) GO TO 40
32*     NR=KO+1
```

33* GO TO 45
34* 40 NR=KO+2
35* 45 RMAT(IJK,KO)=A(NP,NR)
36* LT=IRA+ICA+KRA+KCA
37* LZ=MOD(LT,2)
38* Z=1.
39* IF(LZ,NE,0) Z=1.
40* RETURN
41* END

DIAGNOSTICS

TION TIME = .67 CPU SECONDS

```

1*      FUNCTION NDETRM(N,LN,A,D)
2*      M=0
3*      CALL SIMEQ(N,LN+0,A+0,D+0,M)
4*      NDETRM=M
5*      RETURN
6*      END

```

AGNOSTICS

TION TIME = .21 CPU SECONDS

```

1*      FUNCTION NSIMEQ(N,LN,LM,A,B,D,E)
2*      M=1
3*      CALL SIMEQ(N,LN,LM,A,B,D,E,M)
4*      NSIMEQ=M
5*      RETURN
6*      END

```

AGNOSTICS

ION TIME = .21 CPU SECONDS

```

1*      SUBROUTINE SIMEQ(N,LN,LM,A,B,D,E,M)
2*      INTEGER E
3*      EQUIVALENCE (SAVE,ISAVE)
4*      DIMENSION E(LN),A(N,N),B( N+LM)
5*      IF (M.EQ.0) GO TO 15
6*      DO 10 I=1,LN
7*      10 E(I)=I
8*      15 LNM1=LN+1
9*      CALL OVERFL (IBIG)
10*     DO 80 K=1,LNM1
11*     SAVE=1.0
12*     K1=K+1
13*     DO 25 J=K,LN
14*     DO 25 I=K,LN
15*     IF (SAVE=ABS(A(I,J))), 20,25,25
16*     20 SAVE=ABS(A(I,J))
17*     IBIG=I
18*     JBIG=J
19*     25 CONTINUE
20*     IF (K.EQ.IBIG) GO TO 40
21*     D=D
22*     DO 30 J=K,LN
23*     SAVE=A(K,J)
24*     A(K,J)=A(IBIG,J)
25*     30 A(IBIG,J)=SAVE
26*     IF (M.EQ.0) GO TO 40
27*     DO 35 J=1,LM
28*     SAVE=B(K,J)
29*     B(K,J)=B(IBIG,J)

```

```

0*      35 B(IBIG,J)=SAVE
1*      40 IF (K=JBIG) 45,55,45
2*      45 D=D
3*      DO 50 I=1,LN
4*      SAVE=A(I,K)
5*      A(I,K)=A(I,JBIG)
6*      50 A(I,JBIG)=SAVE
7*      IF (M,EQ,0) GO TO 55
8*      ISAVE=E(K)
9*      E(K)=E(JBIG)
10*     E(JBIG)=ISAVE
11*     55 IF (A(K,K)) 60,130,60
12*     60 D=D*A(K,K)
13*     DO 80 I=K1,LN
14*     SAVE=A(I,K)/A(K,K)
15*     DO 65 J=K1,LN
16*     65 A(I,J)=A(I,J)-SAVE*A(K,J)
17*     CALL OVERFL(IBIG)
18*     IF (IBIG=1) 70,125,70
19*     70 IF (M,EQ,0) GO TO 80
20*     DO 75 J=1,LM
21*     75 B(I,J)=B(I,J)-SAVE*B(K,J)
22*     CALL OVERFL(IBIG)
23*     IF (IBIG=1) 80,125,80
24*     80 CONTINUE
25*     IF (A(LN,LN)) 85,130,85
26*     85 IF(LN,NE,1) D=D*A(LN,LN)
27*     CALL OVERFL(IBIG)
28*     IF (IBIG=1) 90,125,90
29*     90 IF (M) 95,120,95
30*     95 DO 110 J=1,LM
31*     B(LN,J)=B(LN,J)/A(LN,LN)
32*     CALL OVERFL(IBIG)
33*     IF (IBIG=1) 100,125,100
34*     100 DO 110 JBIG=1,LNM1
35*     I=LN-JBIG
36*     SAVE=0,
37*     IP1=I+1
38*     DO 105 K=IP1,LN
39*     105 SAVE=SAVE+A(I,K)*B(K,J)
40*     B(I,J)=(B(I,J)-SAVE)/A(I,I)
41*     CALL OVERFL(IBIG)
42*     IF (IBIG=1) 110,125,110
43*     110 CONTINUE
44*     DO 115 K=1,LN
45*     I=E(K)
46*     DO 115 J=1,LM
47*     115 A(I,J)=B(K,J)
48*     120 M=1
49*     RETURN
50*     125 M=2
51*     RETURN
52*     130 M=3
53*     RETURN
54*     END

```

Input Quantities

NF initial ion (usually 1)
 NT total number of ions (usually 3)
 NALPH number of α 's and β 's
 NOF number of f numbers
 $F(I,J,K)$ f numbers
 T electron temperature ($^{\circ}$ K)
 TR radiation temperature ($^{\circ}$ K)
 ALPH α_{ijk}
 BETA β_{ijk}
 T_1 optical thickness at center of line (K7, K8, K9)
 W dilution factor
 XNE number of electrons
 K7)
 K8 } indeces of thick line
 K9
 LAST not used
 LE some ion between NF and NT (usually 2)
 NTAU number of depth points, TAU
 TAU depth points at which optically thick solutions are made
 DIVIDE constant divisor to prevent overflow of A matrix
 NOY number of thick lines other than line (K7, K8, K9)
 IPROB problem identification number
 ILAST = 1 , go to beginning of program and start new problem with new
 temperatures, etc.
 = 2 , start in middle; temperatures remain the same, but new
 T_1 , W, XNE, etc.
 = 3 , change the Y values only.

Input Cards

<u>Card</u>	<u>Format</u>	<u>Content</u>
1	12I6	NF, NT, NALPH, NØF
2, 2a, 2b, etc.	3I6, E12.8	K, J, K, F_{ijk} a set of cards containing one f number and its indeces per card.
3	6E12.8	T, TR
4, 4a, etc.	3I6, 15X, 2E15.8	I, J, K, α_{ijk} , β_{ijk} a set of cards containing α and β for a given ijk for a given temperature.
5	6E12.8	T_1 , W, XNE
6	12I6	K7, K8, K9, LAST, LE, NTAU
7, 7a, etc.	6E12.8	TAU
8	6E12.8	DIVIDE
9	12I6	NØY
10	12I6	IPRØB, IILAST
11	3I6, E12.8	(if needed) $Y_{ijk} = 1.0$ a set of cards equal in number to NØY containing the indeces for thick lines and $Y_{ijk} = 1.0$

Some Other Constants and Variables

TE	sometimes used for T (electron temperature °K)
AL, ALPHA	sometimes used for ALPH
BE, BET	sometimes used for BETA
MA	array containing the serial number of the first level in each ion. That is, $MA_1 = 1$, $MA_2 = 20$, $MA_3 = 30$.
NST	array containing the number of levels in each ion
NL	number of the last ion (=3)
G(I,J)	statistical weight ion i, level j
E(I,J)	energy values in wave numbers above $E_{1,1}$
ZB(I,J)	number of outer shell electrons
EX(I,J,K)	$ E(I,K) - E(I,J) $ in wave numbers
EV(I,J,K)	EZ in electron volts
BØ	$B \text{ at } Te = \frac{2hv^3}{c^2} / (e \frac{hv}{kT} - 1)$
BTR	B at Tr
BØBTR	B_e/B_{Tr}
XE	4.803×10^{-10} , e - elementary charge
PI	3.1416, π
H	6.6256×10^{-27} Planck constant
CL	2.9979×10^{10} velocity of light cm/sec
XK	1.3805×10^{-16} Boltzmann constant
KM	9.1091×10^{-28} electron rest mass
RCH	2.179×10^{-11} , Rydberg constant x Planck constant x velocity of light
PAZ	8.797×10^{-17} , πA_o , A_o - Bohr radius
NØØ	number of rows and columns in A matrix
A(I,J)	element of A matrix (in this case I and J refer to serial number of level: i.e., A(15, 23) is ion 1, level 15, and ion 2, level 4)
NFI	
NFJ	
NFK	storage arrays for the indeces of f_{ijk}

SIMULTANEOUS LINEAR EQUATION

FUNCTION SUBPROGRAM

```
NSIMEQ(N,LN,LM,A,B,D,E)
XSIMEQ(N,LN,LM,A,B,D,E)
NDETRM(N,LN,A,D)
XDETRM(N,LN,A,D)
```

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NSIMEQ NDETRM
XSIMEQ XDETRM

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PURPOSE:

To solve the matrix equation $A \cdot X = B$ for the unknown matrix X . At the same time, this subroutine computes a scaled version of the determinant of the matrix A .

CALLING SEQUENCE:

This subroutine is used with the following calling sequences:

$M = NSIMEQ(N, LN, LM, A, B, D, E)$

or

$M = XSIMEQ(N, LN, LM, A, B, D, E)$

where

N = a fixed point constant or variable whose value must be equal to the maximum value that may be assumed by the subscript I of the matrix $A(I,J)$. This value is identical with the value given in the DIMENSION statement that sets the upper limits for the subscripts of A (see sample program).

LN = a fixed point constant or variable equal to the actual number of rows or columns in matrix A and the number of rows in matrix B .

LM = a fixed point constant or variable equal to the actual number of columns in matrix B .

A = the source program floating point variable used to designate the elements of matrix A , which may be stored by either row or column. The READ and WRITE statements must be written accordingly.

B = the source program floating point variable used to designate the elements of matrix B .

D = a floating point variable whose value serves as a scale factor by which NSIMEQ or XSIMEQ multiplies the value of the determinant of the matrix A . After the execution of the subroutine, D contains the scaled value of the determinant. The determinant is formed in the following manner:

$$D = \prod_{j=1}^{LN} A(1,j) \cdot D$$

NSIMEQ NDETRM
XSIMEQ XDETRM

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i.e., by forming products of successive pivots with the proper sign adjustment to compensate for the row and column interchanges. Unless the value of the determinant is needed, it is best to set D equal to zero.

E = a fixed or floating point variable array of length at least equal to the number of rows or columns of matrix A. In this area NSIMEQ or XSIMEQ keep a record of the column permutations. The contents of E may be erased after return from the sub-program.

M = a fixed point variable which will be assigned the fixed point constants:

1. if the solution was successful
2. if underflow or overflow occurs
3. if the matrix A is singular.

Note: The type statement INTEGER XSIMEQ must appear in the calling program.

METHOD:

1. Mathematical

Solution of the matrix equation $A \cdot X = B$ is accomplished by upper triangularizing the A matrix using a maximum pivot for each reduction step. This entails searching the reduced $(N-K+1) \times (N-K+1)$ A matrix - at the Kth stage of reduction - for the element with the largest absolute value. A row and column interchange is then performed to bring this element into the A_{KK} position. After completion of the triangularization the X matrix is obtained by back substitution.

2. Coding

FORTRAN IV for the UNIVAC 1107.

RESTRICTIONS:

1. The magnitude of N is restricted only by the number of core locations available and depends therefore on the program in which NSIMEQ or XSIMEQ is used.
2. NSIMEQ and XSIMEQ call another subprogram SIMEQ. Therefore, the use of a subprogram or a function named SIMEQ is forbidden in programs that use NSIMEQ, NDETRM, XSIMEQ, or XDETRM.

NOTE: To solve the matrix equation $A \cdot X = B$ for the unknown matrix X, the dimensions of the various matrices must be:

A: $N \times N$
 B: $N \times LM$ $LM \leq N$
 X: $N \times LM$

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NSIMEQ XDETRM
XSIMEQ XDETRM

It is possible for the programs to give a solution to the matrix equation $A \cdot X = B$ with $LM > N$. If a solution to the matrix equation must be obtained with the B matrix having more columns than the order of matrix A, then the dimensions of the various matrices must be as follows:

A: $N \times LM$

B: $N \times LM$

X: $N \times LM$

ERROR RETURN:

Errors detected in the execution of NSIMEQ or XSIMEQ result in normal UNIVAC Monitor error returns.

The status of the overflow trigger is not preserved on entry. On exit, this trigger is in the OFF position.

STORAGE:

The elements of the matrices A and B are stored in FORTRAN IV order. Execution of this subroutine destroys the original A and B matrices.

After a successful exit from this subroutine, the answers or the X matrix replace the original A matrix. This replacement is done according to the scheme:

$A(I,J)$ is replaced by $X(I,J)$

The programmer may choose to use the same floating point subscripted variable to reference the answer that he used to reference the elements of the A matrix, or he may choose to reference the solution by a different subscripted variable. If the latter is the case, this variable will appear in a dimension and equivalence statement. The choice of parameters which appear with this variable in a dimension statement must be chosen in accordance with the following rule:

If $A(I,J)$ is used to reference elements of the original A matrix and $X(I,J)$ is chosen to reference elements of the solution matrix, then those two variables must appear in a dimension statement with the following parameters:

EQUIVALENCE (A,X)

DIMENSION A(N,N),X(N,L)

where

1. \geq number of columns in matrix.

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NSIMEQ NDETRM
XSIMEQ XDETRM

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STORAGE:

NSIMEQ requires 41_8 words of instruction and 4_8 words of data; SIMEQ requires 740_8 words of instruction and 63_8 words of data.

No COMMON storage is used.

NSIMEQ NDETRM
XSIMEQ XDETRM

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PURPOSE:

To evaluate the expression

$$D \times \text{DET}(A)$$

for a given arbitrary square matrix A and some floating point variable D.

CALLING SEQUENCE:

NDETRM or XDETRM should be used with the following calling sequences:

$$M = \text{NDETRM}(N, LN, A, D)$$

or

$$M = \text{XDETRM}(N, LN, A, D)$$

where N, LN, and A are as described under NSIMEQ or XSIMEQ and

D = a floating point variable. Its value will be used to multiply the determinant in accordance with the scheme outlined under METHOD. On exit from the subroutine the original value of D will be replaced by the scaled value of the determinant. In the case of a singular matrix the determinant (D) will be set to zero.

M = a fixed point variable which will be assigned the following values:

1. if the subroutine was successful;
2. if overflow or underflow occurred;
3. if matrix A was singular.

NOTE: The type statement INTEGER XDETRM must appear in the calling program.

METHOD:**1. Mathematical**

NDETRM and XDETRM are function subprograms that cause entry into the SIMEQ subroutine. Entry by NDETRM or XDETRM cause only the triangularization portion of SIMEQ to be used. (See NSIMEQ or XSIMEQ for a description of this process). The manner in which the determinant is computed is as follows: During each level of reduction of the A matrix the expression

$$\prod_{I=1}^{LN} A(I,I) \cdot D$$

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NSIMEQ NDETRM
XSIMEQ XDETRM

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is computed. After the final level of reduction the result is multiplied by the pivot, a_{nn} . Whenever a row or column interchange is required to put a maximum pivot on the diagonal the sign of the above expression is changed. The final expression will then have the correct sign. If the second argument of NDETRM or XDETRM is a 1, the error return M=1 will occur, indicating the matrix A to be singular whether or not $A(I,I)=0$.

2. Coding

FORTRAN IV for the UNIVAC 1107.

RESTRICTIONS:

1. The magnitude of U is restricted only by the number of core locations available and depend therefore on the program in which NSIMEQ or XSIMEQ is used.
2. NSIMEQ and XSIMEQ call another subprogram SIMEQ. Therefore, the use of a subprogram or a function named SIMEQ is forbidden in programs that use NSIMEQ, NDETRM, XSIMEQ, or XDETRM.

STORAGE:

The elements of matrix A must be stored through the use of a FORTRAN doubly subscripted floating point variable. The subscripts must assume only consecutive integer values.

NDETRM requires 32_g words of instruction and 5_g words of data.

No COMMON storage is used.

PROGRAM FOR SOLUTION OF LINE TRANSPORT
EQUATION

1* C BOUND - BOUND CASE
2* C THREE LEVELS AND CONTINUUM
3* C SOLVES FOR N3/N1
4* DOUBLE PRECISION RR1,EM11,G12,G13
5* DOUBLE PRECISION R2,RK,BJ,C12,C21,C13,C31,C23,C32,PK1,PK2,PK3,
6* IP1K,P2K,P3K,P12,P21,P13,P31,P23,P32,D1,D2,D3,PH12,PH21,PH13,PH31,
7* PPH23,PH32,ZX,ZY,EPS,BS,CJ, SJ,WL,WLM,WKL,WKLM,SW,EM12,EM21
8* DOUBLE PRECISION EF

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```

9*      DOUBLE PRECISION T
10*     DOUBLE PRECISION F
11*     DOUBLE PRECISION FX,GX,AX
12*     DOUBLE PRECISION EM,V
13*     DOUBLE PRECISION NOSONI,X,FI,FIX
14*     DOUBLE PRECISION E1,E2,E3,E4,XK
15*     DOUBLE PRECISION Z,ZT,DZ,ST,ZKL,CON,XN1,R1
16*     COMMON/BLK1/T(31),E1(31),E2(31),E3(31),E4(31)
17*     COMMON/BLK2/F(31+31),FI(31,31),WL(31,31),WLM(31,31),XK(31+31),
18*           XL(31+31)
19*     DIMENSION EPS(31),BS(31),BJ(31)
20*     DIMENSION EF(31+31)+X(31)
21*     DIMENSION EM(31+31),JC(31),V(2)
22*     DIMENSION WKLM(31+31),TK(31+31),SW(31+31)
23*     DIMENSION XN(31),FX(31+31)+FIX(31,31),GX(31),AX(31)+RX(31),CJ(31)
24*     DIMENSION WKL(31+31),SJ(31)
25*     DIMENSION Z(31),R1(31),RK(31)+ZKL(31)+XN1(31),XN2(31),XNK(31)
26*     DIMENSION DA(2)
27*     DIMENSION R2(31),XN3(31)
28*     DIMENSION P12(31)+P21(31)+P13(31)+P31(31),P23(31)+P32(31)
29*     DIMENSION XEPS(31),ETA(31),XIOTA(31)
30*     FORMAT(6E12.8)
31*     12 FORMAT(12I6)
32*     15 FORMAT(16+D12.8,E12.8)
33*     20 FORMAT(1H0,I4,2X+1P5E20.7/(7X+5E20.7))
34*     25 FORMAT(13H0UNIT PRODUCT)
35*     CALL DATE(9,DA)
36*     LX = 31
37*     NC = 31
38*     NR = 31
39*     LMAX = 31
40*     DX = 0.5
41*     PI = 3.14159265
42*     TSP = 1.1283792
43*     ENU = 198305.0
44*     C = 2.997925E+10
45*     H = 6.6256E-27
46*     HK = 1.38054E-16
47*     READ(5,12) IR,IEPS
48*     READ(5,15) ND,ZT,XNT
49*     NZ = 6*ND + 1
50*     NZM = NZ - 1
51*     NZP = NZ + 1
52*     READ(5,30)(R1(I),I=1,NZ)
53*     30 FORMAT(5D15.8)
54*     READ(5,30)(R2(I),I=1,NZ)
55*     READ(5,30)(RK(I),I=1,NZ)
56*     IF(IR.GT.1) READ(5,30)(BJ(I),I=1,NZ)
57*     READ(5,10) XM,TCUT,VEL
58*     READ(5,10) TE,XNE,XNU,G1,G2,G3
59*     READ(5,10) BK12,BK21,BK13,BK31,BK23,BK32
60*     READ(5,10) OM12,OM21,OM13,OM31,OM23,OM32
61*     READ(5,10) BB12,BB21,BB13,BB31,BB23,BB32
62*     READ(5,10) AP21,AP31,AP32,AB1K,AB2K,AB3K
63*     READ(5,10) AL1,AL2,AL3,BE1,BE2,BE3
64*     READ(5,10) DB1K,DB2K,DB3K,DB1,DB2,DB3
65*     IF(IEPS.EQ.1) READ(5,10) (XEPS(I)+ETA(I),I=1,NZ)
66*     A = (2.0*H*XNU**2)*(XNU/(C**2))

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```

67* HKT = (H*XNU)/(HK*TE)
68* SC = A/(EXP(HKT) - 1.0)
69* BET = EXP(-HKT)
70* C12 = XNE*OM12
71* C21 = XNE*OM21
72* C13 = XNE*OM13
73* C31 = XNE*OM31
74* C23 = XNE*OM23
75* C32 = XNE*OM32
76* PK1 = XNE*(AL1 + BE1 + XNE*DB1)
77* PK2 = XNE*(AL2 + BE2 + XNE*DB2)
78* PK3 = XNE*(AL3 + BE3 + XNE*DB3)
79* P1K = AB1K + XNE*QB1K
80* P2K = AB2K + XNE*QB2K
81* P3K = AB3K + XNE*QB3K
82* GO TO (31+36),IR
83* 31 DO 32 I = 1,NZ
84* P12(I) = BB12 + C12
85* P21(I) = BB21 + C21 + AP21
86* P13(I) = BB13 + C13
87* P31(I) = BB31 + C31 + AP31
88* P23(I) = BB23 + C23
89* P32(I) = BB32 + C32 + AP32
90* 32 CONTINUE
91* GO TO 41
92* 36 DO 37 I = 1,NZ
93* P12(I) = C12 + BK12*BJ(I)
94* P21(I) = AP21 + C21 + BK21*BJ(I)
95* P13(I) = C13 + BK13*BJ(I)
96* P31(I) = AP31 + C31 + BK31*BJ(I)
97* P23(I) = C23 + BK23*BJ(I)
98* P32(I) = C32 + AP32 + BK32*BJ(I)
99* 37 CONTINUE
100* 41 CONTINUE
101* D1 = PK1 + PK2
102* D2 = PK1 + PK3
103* D3 = PK2 + PK3
104* PH12 = (P1K*PK2)/D1
105* PH21 = (P2K*PK1)/D1
106* PH13 = (P1K*PK3)/D2
107* PH31 = (P3K*PK1)/D2
108* PH23 = (P2K*PK3)/D3
109* PH32 = (P3K*PK2)/D3
110* G12 = G1/G2
111* G13 = G1/G3
112* IF(IEPS.EQ.1,AND,IR.EQ.1) GO TO 43
113* DO 42 I = 1,NZ
114* EM12 = -(P32(I) + PH32)
115* EM21 = -(P23(I) + PH23)
116* EM11 = P21(I) + PH21 - EM21
117* RR1 = P12(I) + PH12
118* ZX = (C31 + PH31 + P32(I) + PH32 - (EM12*EM21/EM11))/AP31
119* ZY = (G13/AP31)*(C13 + PH13 - EM21*RR1/EM11)
120* EPS(I) = ZX - ZY
121* BS(I) = (A*ZY)/EPS(I)
122* 42 CONTINUE
123* GO TO 46
124* 43 DO 44 I = 1,NZ

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125* EPS(I) = XEPS(I) + ETAC(I)
126* BS(I) = (XEPS(I)*SC + XIOTAC(I))/EPS(I)
127* 44 CONTINUE
128* 46 CONTINUE
129* SQ = (2.0*HK*TE)/XM + VEL**2
130* DNUD = (XNU/C)*SQRT(SQ)
131* PHIZ = 1.0/(DNUD*SQRT(PI))
132* CON = ((H*XNU)/(4.0*PI))*PHIZ*RK13
133* DO 35 I=1,NZ
134* XN1(I) = XNT/(1.0 + R1(I) + R2(I) + RK(I))
135* XN2(I) = R1(I)*XN1(I)
136* XN3(I) = R2(I)*XN1(I)
137* XNK(I) = RK(I)*XN1(I)
138* ZKL(I) = CON*XN1(I)*(1.0 - G13*R2(I))
139* 35 CONTINUE
140* ZTL = 1.000001*ZT
141* ZL = ALOG10(ZTL)
142* KL = ZL
143* LL = KL - ND
144* Z(1) = 0.0
145* Z(2) = 10.0**LL
146* Z(3) = 2.0*Z(2)
147* Z(4) = 5.0*Z(2)
148* NDH = 3*ND + 1
149* NDHP = NDH + 1
150* IF (ND, EQ, 1) GO TO 45
151* DO 40 I=5,NDH
152* Z(I) = 10.0*Z(I-3)
153* 40 CONTINUE
154* 45 DO 50 J=NDHP,NZ
155* JJ = NZ - J + 1
156* Z(J) = ZT + Z(JJ)
157* 50 CONTINUE
158* ST = 0.0
159* T(1) = Z(1)
160* DO 55 I=2,NZ
161* DZ = Z(I) - Z(I-1)
162* T(I) = ST + 0.5*DZ*(ZKL(I-1) + ZKL(I))
163* ST = T(I)
164* 55 CONTINUE
165* WRITE (6,60)(T(J),J=1,NZ)
166* 60 FORMAT(4HOTAU/(1PD30.18))
167* WRITE (6,65)
168* 65 FORMAT(19H1BOUND = BOUND CASE,10X,26HTHREE LEVELS AND CONTINUUM,10
169* 1X,18HSOLUTION FOR N3/N1)
170* WRITE (6,70)DA,ND,ZT,XNT
171* 70 FORMAT(11H0INPUT DATA,100X,A6,A3//20H NUMBER OF DECADES =I3/18H GEI
172* 10METRIC DEPTH =1PE8,1/18H TOTAL PARTICLES =E11.4)
173* WRITE(6,75) XM,VEL
174* 75 FORMAT(4H M =1PE11.4/4H V =E11.4)
175* WRITE (6,80)TCUT
176* 80 FORMAT(7H TCUT =F6.1)
177* WRITE (6,85)(Z(I)+R1(I)+R2(I)+RK(I),XN1(I)+XN2(I)+XN3(I)+XNK(I)
178* 11,NZ)
179* 85 FORMAT(1H0,8X,1HZ,13X,5HN2/N1,10X,5HN3/N1+10X,5HNK/N1,11X,2HN1,13X
180* 1+2HN2+13X+2HN3,13X,2HNK//(1P8E15.4))
181* WRITE(6,86) (Z(I)+ZKL(I)+T(I)+BJ(I),EPS(I),BS(I),I=1,NZ)
182* 86 FORMAT(1H0,8X,1HZ+12X,5HKAPPA+11X+3HTAU+12X,4HJBAR,11X,3HEPS,13X+2

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183*      1HBS/(1P6E15.4))
184*      WRITE (6,95) TE,XNE,XNU,G1,G3
185*      95 FORMAT(5H1TE =1PE22.1/5H NE =E22.4/7H NU31 =E20.5,8H (1/SEC)/7H WT
186*          1 1 =0PF20.0/7H WT 3 =F20.0)
187*          WRITE (6,100) OM12,OM21,OM13,OM31,OM23,OM32
188*      100 FORMAT(12H OMEGA(12) =1PE15.4/12H OMEGA(21) =E15.4/12H OMEGA(13) =
189*          1E15.4/12H OMEGA(31) =E15.4/12H OMEGA(23) =E15.4/12H OMEGA(32) =E15.
190*          2.4)
191*          WRITE (6,105) BB12,BB21,BB13,BB31,BB23,BB32
192*      105 FORMAT(11H BBAR(12) =1PE16.4/11H BBAR(21) = E16.4/11H BBAR(13) =E1
193*          16.4/11H BBAR(31) =E16.4/11H BBAR(23) =E16.4/11H BBAR(32) =E16.4)
194*          WRITE (6,110) AP21,AP31,AP32,AB1K,AB2K,AB3K
195*      110 FORMAT(9H AP(21) =1PE18.4/9H AP(31) =E18.4/9H AP(32) =E18.4/11H AB
196*          1AR(1K) =E16.4/11H ABAR(2K) =E16.4/11H ABAR(3K) =E16.4)
197*          WRITE (6,115) AL1,AL2,AL3,BE1,BE2,BE3
198*      115 FORMAT(12H ALPHA(11) =1PE15.4/12H ALPHA(21) =E15.4/12H ALPHA(31) =
199*          1E15.4/11H BETA(11) =E16.4/11H BETA(21) =E16.4/11H BETA(31) =E16.4)
200*          WRITE (6,120) OB1K,OB2K,OB3K,DB1,DB2,DB3
201*      120 FORMAT(11H DBAR(1K) =1PE16.4/11H DBAR(2K) =E16.4/11H DBAR(3K) =E16.
202*          1.4/11H DBAR(1K) =E16.4/11H DBAR(2K) =E16.4/11H DBAR(3K) =E16.4)
203*          WRITE(6,97) BK12+BK21,BK13,BK31+BK23,BK32
204*      97 FORMAT(6H B12 =1PE21.4/6H B21 =E21.4/6H B13 =E21.4/6H B31 =E21.4/6
205*          1H B23 =E21.4/6H B32 =E21.4)
206*          WRITE(6,125) A,BET,SC
207*      125 FORMAT(4H0A =1PE23.7/4H B =E23.7/9H PLANCK =F18,7)
208*          WRITE(6,98) PK1,PK2,PK3,P1K,P2K,P3K,D1,D2,D3,PH12,PH21,PH13,PH31,
209*          1PH23,PH32
210*      98 FORMAT(6H PK1 =1PE21.4/6H PK2 =E21.4/6H PK3 =E21.4/6H P1K =E21.4/6
211*          1H P2K =E21.4/6H P3K =E21.4/5H D1 =E22.4/5H D2 =E22.4/5H D3 =E22.4/
212*          27H PH12 =E20.4/7H PH21 =E20.4/7H PH13 =E20.4/7H PH31 =E20.4/7H PH2
213*          33 =E20.4/7H PH32 =E20.4)
214*          WRITE(6,99) (Z(I),P12(I),P21(I),P13(I),P31(I),P23(I),P32(I),I=1,NZ
215*          1)
216*      99 FORMAT(1H0,8X,1HZ,13X,3HP12+12X+3HP21+12X+3HP13,12X+3HP31+12X+3HP2
217*          13,12X,3HP32//(1P7E15.4))
218*          NT = NZ
219*          NTM = NT + 1
220*          READ (5,10) YA,YB
221*          IF (T(NZ).LE.1.0) GO TO 440
222*          XA = DLOG(T(NZ))
223*          XMAX = SQRT(XA)
224*          JX = XMAX/DX
225*          NX = JX + 2
226*          XN(1) = 0.0
227*          DO 130 J=2,NX
228*          XJ = J - 1
229*          XN(J) = DX*XJ
230*      130 CONTINUE
231*          WRITE (6,135)(XN(K),K=1,NX)
232*      135 FORMAT(5H0X(K)//(1PE15.2))
233*          DO 140 I=1,NX
234*          DO 140 J=1,NX
235*          FX(I,J) = 0.0
236*          FIX(I,J) = 0.0
237*      140 CONTINUE
238*          DO 145 I=1,NX
239*          FX(I,1) = 1.0
240*          FIX(I,1) = 1.0

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241*      145 CONTINUE
242*          DO 150 J=2,NX
243*              JM = J - 1
244*              DO 150 I=1,JM
245*                  XX = XN(I)/XN(J)
246*                  FX(I,J) = (1.0 - XX)*(1.0 - YA*XX)
247*                  FIX(I,J) = FX(I,J)
248*      150 CONTINUE
249*          IE = NOSONI(FIX,X,NX,LX)
250*          IF (IE.EQ.0) GO TO 425
251*          WRITE (6,155)
252*      155 FORMAT(5H0F(X))
253*          DO 160 I=1,NX
254*              WRITE (6,20) I,(FX(I,J),J=1,NX)
255*      160 CONTINUE
256*          WRITE (6,165)
257*      165 FORMAT(11H0FX INVERSE)
258*          DO 170 I=1,NX
259*              WRITE (6,20) I,(FIX(I,J),J=1,NX)
260*      170 CONTINUE
261*          DO 175 I=1,NX
262*          DO 175 J=1,NX
263*              EF(I,J) = 0.0
264*      175 CONTINUE
265*          DO 180 I=1,NX
266*          DO 180 J=1,NX
267*              EF(I,J) = 0.0
268*          DO 180 K=1,NX
269*              EF(I,J) = EF(I,J) + FX(I,K)*FIX(K,J)
270*      180 CONTINUE
271*          WRITE (6,25)
272*          DO 185 I=1,NX
273*              WRITE (6,20) I,(EF(I,J),J=1,NX)
274*      185 CONTINUE
275*          GX(1) = XN(NX)
276*          DO 190 J=2,NX
277*              GX(J) = 0.5*XN(J)*(1.0 - YA/3.0)
278*      190 CONTINUE
279*          WRITE (6,195) YA,YB
280*      195 FORMAT(5H0YA =1PE11.4/5H YB =E11.4)
281*          DO 200 K=1,NX
282*              AX(K) = 0.0
283*          DO 200 J=1,NX
284*              AX(K) = AX(K) + GX(J)*FIX(J,K)
285*      200 CONTINUE
286*          WRITE (6,205)(XN(I),GX(I),AX(I),I=1,NX)
287*      205 FORMAT(1H0,11X,1HX,18X+4HG(X)+17X,2HAK/(1P3E20.8))
288*          NTK = NZ
289*          NTKM = NTK - 1
290*          DO 210 M=1,NX
291*              X2 = XN(M)**2
292*              EX2 = EXP(-X2)
293*          DO 210 L=1,NZ
294*              TK(L,M) = T(L)*EX2
295*      210 CONTINUE
296*          DO 215 I=1,NX
297*              EX = XN(I)**2
298*              RX(I) = AX(I)*EXP(-EX)

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99*
215 CONTINUE
  DO 220 I=1,NZ
  IT = I
  IF (T(I)=1.0) 220,225,225
301*
302*
303* 220 CONTINUE
304*   ITM = IT
305*   GO TO 230
306* 225 CONTINUE
307*   ITM = IT = 1
308* 230 CONTINUE
309*   DO 235 I=1,NZ
310*   IS = I
311*   IF (T(I)=0.5) 235,235,240
312* 235 CONTINUE
313*   ISM = IS
314*   GO TO 245
315* 240 CONTINUE
316*   ISM = IS = 1
317* 245 CONTINUE
318*   KN = 1
319*   DO 250 I=1,LMAX
320*   DO 250 J=1,LMAX
321*   SW(I,J) = 0.0
322* 250 CONTINUE
C          OUTER LOOP ON FREQUENCY --- INDEX K
323*   DO 320 K=1,NX
324*   KK = K
325*   DO 255 I=1,NZ
326*   T(I) = TK(I,K)
327*
328* 255 CONTINUE
329*   NTK = NZ
330*   NTKM = NTK = 1
331*   TSPR = TSP*RX(K)
332*   WRITE (6,260) XN(K),TSPR
333* 260 FORMAT(4H1X #F6.2,10X,7HCONST =1PE11.4)
334*   WRITE (6,265)(TK(I,K),I=1,NTK)
335* 265 FORMAT(1H0,11X,2HTK//(1PE20.7))
336*   CALL WMAT(NZ*TCUT)
337*   DO 270 I=1,NTK
338*   DO 270 J=1,NTK
339*   WKLM(I,J) = WLM(I,J)
340*   WKL(I,J) = WL(I,J)
341*
342* 270 CONTINUE
343* 275 CONTINUE
344*   IF (IT,EQ,1) GO TO 285
345*   DO 280 I=1,ITM
346*   DO 280 J=1,NZ
347*   SW(I,J) = SW(I,J) + TSPR*WKL(I,J)
348*
349* 280 CONTINUE
350* 285 IF (IT,EQ,NZ) GO TO 295
351*   DO 290 I=IT,NZ
352*   DO 290 J=1,NZ
353*   SW(I,J) = SW(I,J) + TSPR*WKLM(I,J)
354*
355* 290 CONTINUE
356* 295 CONTINUE
357*   WRITE (6,300)
358* 300 FORMAT(17H0WIJK(LAMBDA = 1))
359*   DO 305 I=1,NZ

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357*      WRITE (6,20) I,(WKLH(I,J),J=1,NZ)
358*      305 CONTINUE
359*      WRITE (6,310)
360*      310 FORMAT(13H0WIJK(LAMBDA))
361*      DO 315 I=1,NZ
362*      WRITE (6,20) I,(WKL(I,J),J=1,NZ)
363*      315 CONTINUE
364*      320 CONTINUE
365*      WRITE (6,325)
366*      325 FORMAT(7H0S(I,J))
367*      DO 330 I=1,NZ
368*      WRITE (6,20) I,(SW(I,J),J=1,NZ)
369*      330 CONTINUE
370*      IF (IT,EQ,1) GO TO 340
371*      DO 335 I=1,ITM
372*      DO 335 J=1,NZ
373*      EM(I,J) = -(1.0/(1.0 + EPS(I)))*SW(I,J)
374*      IF(I,EQ,J) EM(I,J) = EM(I,J) + 1.0
375*      335 CONTINUE
376*      340 IF (IT,EQ,NZ) GO TO 350
377*      DO 345 I=IT,NZ
378*      DO 345 J=1,NZ
379*      EM(I,J) = -(1.0/EPS(I))*SW(I,J)
380*      IF(I,EQ,J) EM(I,J) = EM(I,J) + 1.0
381*      345 CONTINUE
382*      350 CONTINUE
383*      IF (IT,EQ,1) GO TO 360
384*      DO 355 I=1,ITM
385*      CJ(I) = (EPS(I)/(1.0 + EPS(I)))*BS(I)
386*      355 CONTINUE
387*      IF (IT,EQ,NZ) GO TO 370
388*      360 DO 365 I=IT,NZ
389*      CJ(I) = BS(I)
390*      365 CONTINUE
391*      370 CONTINUE
392*      DO 375 I=1,NZ
393*      EM(I,NZP) = CJ(I)
394*      375 CONTINUE
395*      WRITE (6,380)
396*      380 FORMAT(7H0M(I,J))
397*      DO 385 I=1,NZ
398*      WRITE (6,20) I,(EM(I,J),J=1,NZP)
399*      385 CONTINUE
400*      N = NZ
401*      MC = NZP
402*      V(1) = 4
403*      CALL GJR(EM,NC,NR,N,MC,8410,JC,V)
404*      DO 390 I=1,NZ
405*      SJ(I) = EM(I,NZP)
406*      BJ(I) = SJ(I)*(1.0 + EPS(I)) + EPS(I)*BS(I)
407*      ZY = EPS(I)*BS(I)/A
408*      ZX = EPS(I) + ZY
409*      RR1 = P12(I) + PH12
410*      EM12 = -(P32(I) + PH32)
411*      EM11 = P21(I) + PH21 + P23(I) + PH23
412*      R2(I) = (G3/G1)*(BJ(I)/A + ZY)/(1.0 + BJ(I)/A + ZX)
413*      R1(I) = (RR1 - R2(I)*EM12)/EM11
414*      RK(I) = (P1K + R1(I)*P2K + R2(I)*P3K)/(PK1 + PK2 + PK3)

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015*      390 CONTINUE
016*      PUNCH 395*(R1(J),J=1,NZ)
017*      PUNCH 395*(R2(I),I=1,NZ)
018*      PUNCH 395*(RK(J),J=1,NZ)
019*      PUNCH 395*(BJ(J),J=1,NZ)
020*      395 FORMAT(5E15.8)
021*      WRITE (6,400)(Z(J)+SJ(J),BJ(J),R1(J),R2(J),RK(J),J=1,NZ)
022*      400 FORMAT(1H0,13X,1HZ+19X,1HS,19X,1HJ,17X,5HN2/N1,15X,5HN3/N1,15X,5HN
023*                  1K/N1//(1P6E20.4))
024*      405 CALL EXIT
025*      410 WRITE (6,415)
026*      415 FORMAT(21H0ERROR IN EQ. SOLVING)
027*      WRITE (6,420)NC,NR,N,MC,V
028*      420 FORMAT(5H0NC =I3.5X,4HNR =I3.5X,3HN =I3.5X,4HMC =I3.5X,4HV1 =I8.1
029*                  1.5X,4HV2 =E11.4)
030*      GO TO 405
031*      425 WRITE (6,430)IE,NX
032*      430 FORMAT(14H0ERROR IN F(X)/5H IE =I3.5X,4HNX =I3)
033*      WRITE (6,155)
034*      DO 435 I=1,NX
035*      WRITE (6,20)I,(FX(I,J),J=1,NX)
036*      435 CONTINUE
037*      GO TO 405
038*      440 WRITE (6,445)T(NT)
039*      445 FORMAT(20H0TAU-MAX TOO SMALL =1PE11.4)
040*      GO TO 405
041*      END

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DIAGNOSTICS

UTION TIME = 8.23 CPU SECONDS

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1*      SUBROUTINE WMAT(NZ,TCUT)
2*      C      CALCULATES W(LAMBDA) AND WL(LAMBDA = 1) AT LINE CENTER
3*      DOUBLE PRECISION WL,WLM
4*      DOUBLE PRECISION T,E1,E2,E3,E4,A1,A2,A3,A4,A5,ESB,B1,B2,B3
5*      DOUBLE PRECISION F,FI,XK
6*      COMMON/BLK1/T(31),E1(31),E2(31),E3(31),E4(31)
7*      COMMON/BLK2/F(31*31),FI(31,31),WL(31,31),WLM(31,31),XK(31*31),
8*                  1XL(31*31)
9*      10 FORMAT(1H0,I4,2X+1P5E20.7/(7X,5E20.7))
10*      NT = NZ
11*      DO 15 I=1,NZ
12*      DO 15 J=1,NZ
13*      WL(I,J) = 0.0
14*      WLM(I,J) = 0.0
15*      15 CONTINUE
16*      NM = NZ - 1
17*      DO 25 I=1,NM
18*      JP = I + 1
19*      DO 20 J=JP,NM
20*      A1 = DABS(T(J-1)-T(I))

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21* IF (A1,GT,TCUT) GO TO 25
22* A2 = DABS(T(J) - T(I))
23* A3 = DABS(T(J+1) - T(I))
24* A4 = T(J) - T(J-1)
25* A5 = T(J+1) - T(J)
26* B1 = (T(I)*(ESB(A1,2) - ESB(A2,2)) + DEXP(-A1) - DEXP(-A2)
27* 1 + ESB(A2+3) - ESB(A1,3))/A4
28* B2 = (T(J+1)/A4)*(ESB(A1,2) - ESB(A2,2)) - (T(J+1)/A5)*(ESB(A2,2)
29* 1 - ESB(A3,2))
30* B3 = (T(I)*(ESB(A2,2) - ESB(A3,2)) + DEXP(-A2) - DEXP(-A3)
31* 1 + ESB(A3,3) - ESB(A2,3))/A5
32* WL(I,J) = 0.5*(B1 + B2 + B3)
33* WLM(I,J) = WL(I,J)
34* 20 CONTINUE
35* 25 CONTINUE
36* DO 35 J=2,NM
37* IP = J + 1
38* DO 30 I=IP,NZ
39* A3 = DABS(T(I) - T(J+1))
40* IF (A3,GT,TCUT) GO TO 35
41* A1 = DABS(T(I) - T(J-1))
42* A2 = DABS(T(I) - T(J))
43* A4 = T(J) - T(J-1)
44* A5 = T(J+1) - T(J)
45* B1 = (A1/A4)*(ESB(A2,2) - ESB(A1,2)) + ((T(J+1) - T(I))/A5)*(
46* 1 ESB(A3,2) - ESB(A2,2))
47* B2 = (DEXP(-A3) - DEXP(-A2) + ESB(A2,3) - ESB(A3,3))/A5
48* B3 = (DEXP(-A2) - DEXP(-A1) + ESB(A1,3) - ESB(A2,3))/A4
49* WL(I,J) = 0.5*(B1 + B2 + B3)
50* WLM(I,J) = WL(I,J)
51* 30 CONTINUE
52* 35 CONTINUE
53* DO 40 I=2,NM
54* A1 = T(I) - T(I-1)
55* A2 = T(I+1) - T(I)
56* B1 = 2.0 - ESB(A1,2) - ESB(A2,2)
57* B2 = (0.5 - DEXP(-A1) + ESB(A1,3))/A1
58* B3 = (0.5 - DEXP(-A2) + ESB(A2,3))/A2
59* WL(I,I) = 0.5*(B1 + B2 + B3)
60* WLM(I,I) = WL(I,I) = 1.0
61* 40 CONTINUE
62* DO 45 I=1,NM
63* A1 = DABS(T(NM)-T(I))
64* IF (A1,GT,TCUT) GO TO 45
65* A2 = DABS(T(NZ) - T(I))
66* A3 = T(NZ) - T(NM)
67* B1 = (T(I)*(ESB(A1,2) - ESB(A2,2)) + DEXP(-A1) - DEXP(-A2)
68* 1 + ESB(A2+3) - ESB(A1,3))/A3
69* B2 = (T(NM)/A3)*(ESB(A1,2) - ESB(A2,2))
70* WL(I,NZ) = B1 + B2
71* WLM(I,NZ) = WL(I,NZ)
72* 45 CONTINUE
73* A3 = T(2) - T(1)
74* DO 50 I=2,NZ
75* A2 = DABS(T(2) - T(I))
76* IF (A2,GT,TCUT) GO TO 50
77* A1 = DABS(T(1) - T(I))
78* B1 = ((T(2) - T(I))/A3)*(ESB(A2,2) - ESB(A1,2))

```

```

79*      B2 = (DEXP(-A2) + DEXP(-A1) + ESB(A1,3) + ESB(A2,3))/A3
80*      WL(I+1) = 0.5*(B1 + B2)
81*      WLM(I+1) = WL(I,1)
82* 50 CONTINUE
83*      IF (A3.GT.TCUT) GO TO 55
84*      WL(1+1) = 0.5*(1.0 + ESB(A3,2) + (0.5 - DEXP(-A3) + ESB(A3,3))/A3)
85*      GO TO 60
86*      55 WL(1+1) = 0.5 - (0.25/A3)
87*      60 WLM(1+1) = WL(1+1) - 1.0
88*      A1 = T(NZ) = T(NM)
89*      IF (A1.GT.TCUT) GO TO 65
90*      WL(NZ,NZ) = 0.5*(1.0 - ESB(A1,2) - (0.5 - DEXP(-A1) + ESB(A1,3))
91*           1 /A1)
92*      GO TO 70
93*      65 WL(NZ,NZ) = 0.5 - (0.25/A1)
94*      70 WLM(NZ,NZ) = WL(NZ,NZ) - 1.0
95*      WRITE (6,75)
96*      75 FORMAT(10H0W(LAMBDA))
97*      DO 80 I=1,NT
98*      WRITE (6,10) I,(WL(I,J),J=1,NT)
99* 80 CONTINUE
100*      WRITE (6,85)
101*      85 FORMAT(14H0W(LAMBDA = 1))
102*      DO 90 I=1,NT
103*      WRITE (6,10) I,(WLM(I,J),J=1,NT)
104* 90 CONTINUE
105*      RETURN
106*      END

```

DIAGNOSTICS

UTION TIME = 2.60 CPU SECONDS

```

1*      SUBROUTINE GJR(A,NC,NR,N,M0,S,JC,V)
2*      DOUBLE PRECISION A,X,V
3*      DIMENSION A(NR,NC),JC(1),V(2)
4*      C
5*      C      JC IS THE PERMUTATION VECTOR
6*      C      KD IS THE OPTION KEY FOR DETERMINANT EVALUATION
7*      C      KI IS THE OPTION KEY FOR MATRIX INVERSION
8*      C      L IS THE COLUMN CONTROL FOR AX=B
9*      C      M IS THE COLUMN CONTROL FOR MATRIX INVERSION
10*     C
11*     C      INITIALIZATION
12*     C
13*     C      IW=V(1)
14*     C      M=1
15*     C      S=1.
16*     C      L=N+(M0-N)*(IW/4)
17*     C      KD=2-MOD(IW/2,2)
18*     C      IF(KD.EQ.1) V(2)=0.
19*     C      KI=2-MOD(IW,2)
20*     C      GO TO (10,20)+KI
21*     C
22*     C      INITIALIZE JC FOR INVERSION
23*     C
24*     C      10 DO 15 I=1,N
25*     C      15 JC(I)=I

```

```

26* C
27* C      SEARCH FOR PIVOT ROW
28* C
29* 20 DO 85 I=1,N
30* GO TO (30,25),KI
31* 25 M=I
32* 30 IF (I,EQ,N) GO TO 55
33* X=1.
34* DO 35 J=I,N
35* IF (X,GT,ABS(A(J,I))) GO TO 35
36* X = DABS(A(J,I))
37* K=J
38* 35 CONTINUE
39* IF (K,EQ,I) GO TO 55
40* S=S
41* V(1)=V(1)
42* GO TO (40,45),KI
43* 40 MU=JC(I)
44* JC(I)=JC(K)
45* JC(K)=MU
46* C
47* C      INTERCHANGE ROW I AND ROW K
48* C
49* 45 DO 50 J=M,L
50* X=A(I,J)
51* A(I,J)=A(K,J)
52* 50 A(K,J)=X
53* C
54* C      TEST FOR SINGULARITY
55* C
56* 55 IF (DABS(A(I,I)),GT,0.0) GO TO 60
57* C
58* C      MATRIX IS SINGULAR
59* C
60* IF(KD,EQ,1) V(1)=0.
61* JC(1)=I-1
62* RETURN 6
63* 60 GO TO (65,70),KD
64* C
65* C      COMPUTE THE DETERMINANT
66* C
67* 65 IF(A(I,I),LT,0.) S=S
68* V(2) = V(2) + DLLOG(DABS(A(I,I)))
69* 70 X=A(I,I)
70* A(I,I)=1.
71* C
72* C      REDUCTION OF THE I-TH ROW
73* C
74* DO 75 J=M,L
75* A(I,J)=A(I,J)/X
76* C
77* C      TEST OVERFLOW SWITCH, IF ON
78* RETURN NEGATIVE VALUE OF I IN JC(1)
79* C
80* CALL OVERFL (IFL)
81* IF (IFL,EQ,1) GO TO 120
82* 75 CONTINUE
83* C

```

```

84*   C      REDUCTION OF ALL REMAINING ROWS
85*   C
86*   DO 85 K=1,N
87*   IF (K,EQ,I) GO TO 85
88*   X=A(K,I)
89*   A(K,I)=0.
90*   DO 80 J=M,L
91*   A(K,J)=A(K,J)-X*A(I,J)
92*   C
93*   C      TEST OVERFLOW SWITCH. IF ON
94*   C      RETURN NEGATIVE VALUE OF I IN JC(1)
95*   C
96*   CALL OVERFL (IFL)
97*   IF (IFL,EQ,1) GO TO 120
98*   80 CONTINUE
99*   85 CONTINUE
100*  C
101*  C      AX=B AND DET.(A) ARE NOW COMPUTED
102*  C
103*  GO TO (90,115),KI
104*  C
105*  C      PERMUTATION OF THE COLUMNS FOR MATRIX INVERSION
106*  C
107*  90 DO 110 J=1,N
108*  IF (JC(J),EQ,J) GO TO 110
109*  JJ=J+1
110*  DO 95 I=JJ,N
111*  IF (JC(I),EQ,J) GO TO 100
112*  95 CONTINUE
113*  100 JC(I)=JC(J)
114*  DO 105 K=1,N
115*  X=A(K,I)
116*  A(K,I)=A(K,J)
117*  105 A(K,J)=X
118*  110 CONTINUE
119*  115 JC(1)=N
120*  IF (KD,EQ,1) V(1)=S
121*  RETURN
122*  120 JC(1)=I-I
123*  IF (KD,EQ,1) V(1)=S
124*  RETURN 6
125*  END

```

IAGNOSTICS

TION TIME = 2.00 CPU SECONDS

```

1*      DOUBLE PRECISION FUNCTION NOSONI(A,X,L,LMAX)
2*      DOUBLE PRECISION A,X,F
3*      DIMENSION A(1),X(1)
4*      N = L = 1
5*      MAX = N*LMAX + L
6*      MAX = N*LMAX + L
7*      DO 10 I=1,L
8*      X(I) = 1.0
9* 10 CONTINUE
10*     K1 = -LMAX
11*     DO 55 K=1,L
12*     K1 = K1 + LMAX
13*     K2 = K1 + K
14*     IF (A(K2)) 15,80+15
15* 15 DO 30 I=1,L
16*     J1 = K1 + I
17*     IF (A(J1)) 20,30+20
18* 20 F = 1.0/A(J1)
19*     X(I) = X(I)*F
20*     DO 25 J1=I,MAX,LMAX
21*     A(J1) = A(J1)*F
22* 25 CONTINUE
23* 30 CONTINUE
24*     A(K2) = X(K)
25*     X(K) = 1.0
26*     DO 50 I=1,L
27*     K1 = K - I
28*     IF (K1) 35,50,35
29* 35 J1 = K1 + I
30*     IF (A(J1)) 40,50+40
31* 40 A(J1) = 0.0
32*     DO 45 J2=I,MAX,LMAX
33*     J1 = J2 + K1
34*     A(J2) = A(J2) - A(J1)
35* 45 CONTINUE
36* 50 CONTINUE
37* 55 CONTINUE
38*     DO 70 I=1,N
39*     IF (X(I)) 60,80,60
40* 60 F = 1.0/X(I)
41*     DO 65 J1=I,MAX,LMAX
42*     A(J1) = A(J1)*F
43* 65 CONTINUE
44* 70 CONTINUE
45*     NOSONI = 1
46* 75 RETURN
47* 80 NOSONI = 0
48*     GO TO 75
49*     END

```

DIAGNOSTICS

ATION TIME = .93 CPU SECONDS

INPUT DEFINITIONS

General

IR = 1 at initial start
 2 for iteration
 IEPS = 1, ϵ_i' , η_i and ℓ_i are read in from P48 (Code 1)
 IEPS \neq 1, ϵ_i , η_i and ℓ_i are calculated
 ND = number of decades (max. = 5)
 ZT = geometric thickness
 XNT = total number density
 R1 = n_2/n_1
 R2 = n_3/n_1
 RK = n_k/n_1
 BJ = \bar{J}_c (input on iteration)
 XM = mass of Helium = 6.6408×10^{-24} g
 VEL = non-thermal velocity in Doppler width
 TCUT = upper limit on optical depth to avoid overflow in exponential routines
 TE = $T_e(^{\circ}\text{K})$
 XNE = n_e
 XNU = $v_{ij} (1/\text{sec}) (= c \times 10^8 / \lambda_{ij})$, λ_{ij} from program 48 (Code 1)
 G1 =
 G2 = } statistical weights for each level
 G3 =
 YA = constant coefficient in $f(x)_j$ and g_j (usually = 1.0)
 YB = constant coefficient in $f'(y)_j$ and g'_j (usually = 1.0)

Two Level Atom (Bound-Free Case)

DY = increment in y_k
 BIJK = B_{jk} Einstein absorption coefficients - Ion I
 BIKJ = B_{kj} Einstein absorption coefficients - Ion I
 ENU = ΔE_k in wave numbers
 ALPHA = α_{k2}

Two Level Atom (Continued)

BETA = β_{k2}
 ABAR = \bar{A}_{2k}
 OMEGA = Ω_{21}
 OBAR = $\bar{\Omega}_{2k}$
 DBAR = Ω_{k2}
 AP = A_{21}
 BB = $B_{\nu 21}$
 RS = \bar{A}_{1k} at T_e
 OB = $\bar{\Omega}_{1k}$
 XE1 = n_1^*
 XE2 = n_2^*
 XEK = n_k^*
 OM12 = Ω_{12}
 BB12 = $B_{\nu 21}$

Input Card Formats

Card	Format	Content
1	(I6)	IR
2	(I6,2E12.8)	ND, ZT, XNT
3	(6E12.8)	TCUT
4,4a, etc.	(5E15.8)	R _{1i}
5,5a, etc.	"	R _{Ki}
6,6a, etc.	"	B _{Ji} (only on iteration)
7	(6E12.8)	DY, BIJK, BIKJ, ENU
8	"	TE, XNE, ALPHA, BETA, ABAR, OMEGA
9	"	OBAR, DBAR, AP, BB, RS, OB
10	"	XE1, XE2, XEK, OM12, BB12
11	"	YA, YB

Three Level Atom (both n_2/n_1 and n_3/n_1 solutions)

BK_{ij} = Einstein absorption coefficient
 OM_{ij} = Ω_{ij}

Three Level Atom (Continued)

$$\begin{aligned}
 BB_{ij} &= B_j B_{kj} \\
 AP_{ij} &= A_{ij} \\
 AB_{ik} &= \bar{A}_{ik} \\
 AL_i &= \alpha_{k,i} \\
 BE_i &= \beta_{k,i} \\
 OB_{ik} &= \bar{\Omega}_{ik} \\
 DB_i &= \bar{\Omega}_{k,i}
 \end{aligned}$$

Input Card Format

Card	Format	Content
1	(2I6)	IR, IEPS
2	(I6,D12.8,E12.8)	ND, ZT, XNT
3,3a,etc.	(5D15.8)	R1 _i
4,4a,etc.	"	R2 _i
5,5a,etc.	"	RK _i
6,6a,etc.	"	BJ _i
7	(6E12.8)	XM, TCUT, VEL
8	"	TE, XNE, XNU(I,J), G1, G2, G3
9	"	BK12, BK21, BK13, BK31, BK23, BK32
10	"	OM12, OM21, OM13, OM31, OM23, OM32
11	"	BB12, BB21, BB13, BB31, BB23, BB32
12	"	AP21, AP31, AP32, AB1K, AB2K, AB3K
13	"	AL1, AL2, AL3, BE1, BE2, BE3
14	"	OB1K, OB2K, OB3K, DB1, DB2, DB3
15	"	XEPS, ETA, IOTA, XEPS, ETA, IOTA
16	"	YA, YB

OMEGA	Ω_{ijk} , electron collisional excitation coefficient
AP	A_{ijk} , Einstein spontaneous transition probability
BB	B_{ijk} , Einstein absorption transition probability x Planck function
ΦBAR	$\bar{\Omega}_{ijk}$, electron collisional ionization coefficient
DBAR	$\bar{\Lambda}_{ijk}$, electron collisional recombination coefficient
ABAR	Λ_{ijk} , radiative ionization rate
ΦD	optical depth
HH or H	physical thickness of layer (calculated in AMAT)

DEFINITIONS OF OTHER CONSTANTS AND VARIABLES

PI =	$\pi = 3.14159265$
C =	2.997925×10^{10} cm/sec
H =	6.6256×10^{-27} erg s, Planck constant
HK =	1.38054×10^{-16} erg/ $^{\circ}$ K, Boltzmann constant
c_p =	1.8×10^{-18} , 7.6×10^{-18}
TSP =	$1.1283792 = 2/\pi$
Z =	geometric depth
DZ =	increment in Z
T =	table of optical depths at line center
NT =	number of T
TK =	optical depth dependent upon frequency
NTK =	number of TK
X =	$(\nu - \nu_o)/(\Delta\nu_D)$
DX =	increment in X
NX =	number of X
FX =	$f(X)_j$
FIX =	inverse matrix of $f(X)_j$
GX =	g_j
AX =	A_k
Y =	ν/ν_{kl}
DY =	increment in Y
NY =	number of Y
FY =	$f'(y)_j$
FIY =	inverse of $f'(y)_j$
GY =	g'_j
AY =	A'_k
XN1 =	n_1
XN2 =	n_2
XN3 =	n_3
XNK =	n_k
WL =	$w_{ij}(\Lambda)$ at line center
WLM =	$w_{ij}(\Lambda-l)$ at line center

$W_{KL} = W_{ijk}^{(\Lambda)}$ at frequency ν_k
 $W_{KLM} = W_{ijk}^{(\Lambda-1)}$ at frequency ν_k
 $E_1 =$
 $E_2 =$
 $E_3 =$
 $E_4 = \left\{ \begin{array}{l} \\ \\ \text{exponential integrals of orders 1, 2, 3 and 4} \end{array} \right.$
 $P_{ij} = \text{refer to capital } P_{ij}$
 $P_{Hij} = \text{refer to script } P_{ij}$
 $\epsilon_{PS} = \epsilon$
 $B_S = B^S$
 $\epsilon_A = \epsilon^a$
 $\epsilon_B = \epsilon^b$
 $E_M_{ij} = M_{11}, M_{12}, \text{ etc. in deriving X and Y in multi-level case}$

7.7. GJR - Determinant; Inverse; Solution of Simultaneous Equations

7.7.1. Purpose

This subroutine solves simultaneous equations, computes a determinant, or inverts a matrix or any combination of the three above by using a Gauss-Jordan elimination technique with column pivoting.

7.7.2. User Procedure

7.7.2.1. Entry

```
CALL GJR(A,NC,NR,N,MC,$k,JC,V)
```

where:

	DESCRIPTION	TYPE
A	is the matrix whose inverse or determinant is to be determined. If simultaneous equations are to be solved the last MC - N columns of the matrix are the constant vectors of the equations to be solved. On output if the inverse is computed it is stored in the first N columns of A. If simultaneous equations are solved, the last MC - N columns contain the solution vectors.	floating-point array; input and output
NC	is the maximum number of columns of the array A.	FORTRAN integer; input
NR	is the maximum number of rows of the array A.	FORTRAN integer; input
N	is the number of rows of the array A.	FORTRAN integer; input
MC	is the number of columns of the array A. This entry is a dummy argument, if simultaneous equations are not solved.	FORTRAN integer; input
k	is a statement number in the calling program to which control is returned if an overflow is detected. It must be preceded by \$ in the calling sequence.	input
JC	is a one-dimensional permutation array of N elements used for permuting the rows and columns of A if an inverse is computed. If an inverse is not computed this argument must have at least one cell for the error return identification. On output, the first element of the array is N if control is returned normally. If an overflow is	FORTRAN integer array; input and output

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detected, the first element is the negative of the last correctly completed row of the reduction. If matrix singularity is detected, the entry contains the value of the last row before the singularity was detected.

V is a one-dimensional array. If the determinant is not computed it has one entry, otherwise it has two. On input **V(1)** is the option indicator, its values are set as follows:

Operation	V(1)						
	1.	2.	3.	4.	5.	6.	7.
Compute Determinant	no	yes	yes	no	no	yes	yes
Invert Matrix	yes	no	yes	no	yes	no	yes
Solve Equations	no	no	no	yes	yes	yes	yes

On normal return from the program **V(1)** contains the value of the natural logarithm of the absolute value of the determinant and **V(2)** contains the sign of the determinant. If an error return is made, and the determinant was to be computed, then **V(1)** is set to 0 and, if an overflow return was made, **V(2)** contains the sign of the last correct partially-computed value of the determinant.

7.7.2.2. Restrictions

None.

7.7.2.3. Special Considerations

- (1) If the matrix is singular or ill-conditioned, roundoff error may cause large discrepancies in the results.
- (2) In the case of a singular matrix, return may not be made through the singularity exit because of roundoff error.
- (3) See paragraph 7.1.2.3. for notes on usage of the row-dimension in arguments **N** and **NR**.

7.7.2.4. Other Subprograms Required

None.

7.7.2.5. Error Returns

- (1) If a singularity is detected, the first element of the array JC is set to the row number before the singularity was detected and, if the determinant was to be computed the value of V(1) is set to 0.0. Control is then returned to the calling program at the statement number specified.
- (2) If an overflow is detected, JC(1) is set to the negative of the last correctly completed row of the reduction. V(2) is set to the sign of the partial value of the determinant that was computed until this time. Control is then returned to the calling program at the statement number specified.

7.7.3. Supporting Information

7.7.3.1. Mathematical Method

For any matrix A, if a matrix B exists such that $BA = AB = I$ and I is the unit matrix, then $B = A^{-1}$.

If $AX = C$, where A is n by n, X is n by p, and C is n by p, then the solution to these sets of simultaneous equations is

$$X = A^{-1}C$$

The determinant of A is defined by the following equation

$$|A| = \sum (-1)^{f(j_1, \dots, j_n)} \prod_{i=1}^N a_{ij_i}$$

where

a_{ij} is the (i,j) th element of the matrix A.

$f(j_1, \dots, j_n)$ is the number of transpositions required to transform $(1, \dots, n)$ to (j_1, \dots, j_n) ; the summation is over all permutations (j_1, \dots, j_n) of the integers $(1, \dots, n)$.

The solution to all of these problems is found by using a Gauss-Jordan elimination scheme with row scaling and maximal pivoting by columns.

Faddeev, D.K., and Faddeeva, V.N., Computational Methods of Linear Algebra, W.H. Freeman and Co., (1963).

Ralston and Wilf, Numerical Methods for Digital Computers Wiley (1960).

7.7.3.2. Programming Method

- (1) For each column below the diagonal, the program searches for a pivotal element by finding the element of maximum absolute value in the remaining rows of the column.
- (2) This row is interchanged with the row of the diagonal.

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- (3) Each of the elements of the pivotal row is divided by the pivot except the pivot which is replaced by its reciprocal.
- (4) All the other rows of the array are changed by the formula

$$a_{ij} = a_{ij} - a_{ik} \cdot a_{kj}$$

where a_{kk} is the pivotal element. If $i = k$, a_{ij} is replaced by 0.

- (5) When this process has been completed for each diagonal of the array, the columns of the matrix are repermuted to give the inverse in the first N columns of the array A.
- (6) If the determinant is to be found, each permutation of rows and columns changes the value of its sign. The natural logarithm of the absolute value of the diagonal element is summed after step 2.
- (7) Only the computations necessary for the options specified are carried out.

7.7.3.3. Storage

GJR: 470 positions, not including the Library Subroutines OVERFL, ALOG and NERR\$2.

7.7.3.4. Nomenclature

IFL is the overflow test indicator.

IW is the FORTRAN integer value of the option indicator.

KD is the option key for determinant evaluation.

KI is the option key for matrix inversion.

L is the column control for solution of simultaneous equations.

M is the column control for matrix inversion.

MU is a dummy variable.

S is the sign control for determinant evaluation.

X is a dummy variable.

All other variable names used in GJR are either loop indices or are defined in paragraph 7.7.2.1.

7.7.4. Test Design

7.7.4.1. Introduction

The test program reads a matrix and seven options into main storage and successively references GJR for each of the options, thus testing the program's functioning.

7.7.4.2. Comments

The test program computes

$$A^{-1}A = R \approx I$$

after the inverse is found by GJR. This check shows that computational accuracy is better than 4×10^{-8} for all elements of the inverse matrix. However, this accuracy depends on the well-conditioning of the matrix to be inverted.

7.7.4.3. Test Input

The matrix used as a test matrix was symmetric positive definite of order 4 scaled so that each diagonal element is one. See Faddeeva Chapter 2.

Card 1:	Title Card. Col. 1-72	FORMAT (12A6) An alphanumeric heading to be printed by the test program.
Card 2:	Parameter Card. Col. 1-2	FORMAT (3I2,7I5) N, the number of rows of matrix A.
	Col. 3-4	NC, the number of columns of matrix A.
	Col. 5-6	NOP, the number of options to be specified in successive calls to GJR. NOP ≤ 7 .
	Col. 7-11	IOP(1), first option indicator.
	Col. 12-16 : : Col. 71-80	IOP(2) second option indicator. : : IOP(NOP), last option indicator.

Each element of the IOP array appears as V(1) in a separate call to GJR.

Card 3ff:	Matrix Cards. Col. 1-10	FORMAT (8E10.3)
	Col. 11-20 : : Col. 71-80	Elements of A. The NC columns of row 1 are input first, followed by rows 2 through N.

The input data is listed below.

TEST MATRIX 1. (REF. FADDEEVA - COMP.MTHS.OF LINEAR ALGEBRA CHAP.2)

640807	1	2	3	4	5	6	7	
1.	.42		.54		.66		.25	.3
.42		1.		.32		.44		.45
.54			.32		1.		.22	.7
.66			.44			1.		.85

APPENDIX C
PROGRAM FOR SOLUTION OF CONTINUUM TRANSPORT EQUATION

155

For inputs, definitions, and subroutines see Appendix B.

```

1*      C          BOUND = FREE CASE
2*      C          TWO LEVELS AND CONTINUUM
3*      DOUBLE PRECISION FY,FIY
4*      DOUBLE PRECISION T,E1,E2,E3,E4
5*      DOUBLE PRECISION F,FI,XK,EF,X
6*      DOUBLE PRECISION EM,V
7*      DOUBLE PRECISION Z,ZT,DZ,ST,ZKL,XN1
8*      COMMON/BLK1/T(31),E1(31),E2(31),E3(31),E4(31)
9*      COMMON/BLK2/F(31,31),FI(31,31),WL(31,31),WLM(31,31),XK(31,31),
10*     XL(31,31)
11*     DIMENSION RP(31),EM(31,31),B(31),JC(31),V(2)
12*     DIMENSION EF(31,31),X(31)
13*     DIMENSION WKL(31,31),TK(31,31),SW(31,31)
14*     DIMENSION Y(31),FY(31,31),FIY(31,31),GY(31),AY(31)
15*     DIMENSION Z(31),R1(31),RK(31),ZKL(31),XN1(31),XN2(31),XNK(31)
16*     DIMENSION DA(2)
17*     DIMENSION BJ(31),P12(31),P21(31),EA(31),EB(31)
18*     DIMENSION WP(31,31),WKL(31,31),RA(31)
19*     11 FORMAT(I6,D12.8,E12.8)
20*     16 FORMAT(6E12.8)
21*     21 FORMAT(16,2E12.8)
22*     26 FORMAT(1H0,I4,2X,1P5E20.7/(7X,5E20.7))
23*     31 FORMAT(13H0UNIT PROD(I))
24*     CALL DATE(9,DA)
25*     DO 36 I=1,LMAX
26*     DO 36 J=1,LMAX
27*     WP(I,J) = 0.0
28*     SW(I,J) = 0.0

```

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```

29*      36 CONTINUE
30*          NC = 31
31*          NR = 31
32*          LMAX = 31
33*          C = 2.997925E+10
34*          H = 6.6256E-27
35*          HK = 1.38054E-16
36*          PI = 3.1415926
37*          CP = 7.6E-10
38*          READ (5,21) IR
39*          READ (5,11) ND,ZT,XNT
40*          READ (5,16) TCUT
41*          NZ = 6*ND + 1
42*          NZM = NZ - 1
43*          NZP = NZ + 1
44*          READ (5,466)(R1(I),I=1,NZ)
45*          READ (5,466)(RK(I),I=1,NZ)
46*          IF (IR.GT.1) READ (5,466)(BJ(I),I=1,NZ)
47*          READ(5,16) DY,BIJK,BIKJ,ENU
48*          READ (5,16) TE,XNE,ALPHA,BETA,ABAR,OMEGA,UBAR,DBAR,AP,BB,RS,OB
49*          READ (5,16) XE1,XE2,XEK,OM12,BB12
50*          CON = (8.0*PI)*((ENU**3)*CP)*C
51*          THN = H*ENU)*C
52*          THD = HK*TE
53*          TH = THN/THD
54*          C1K = XNE*OB
55*          P2K = ABAR + XNE*UBAR
56*          PK2 = ALPHA + BETA + XNE*DBAR
57*          PK2 = XNE*PK2
58*          GO TO (41+51),IR
59*          41 DO 46 I=1,NZ
60*              P12(I) = BB12 + XNE*OM12
61*              P21(I) = BB + AP + XNE*OMEGA
62*          46 CONTINUE
63*          GO TO 61
64*          51 DO 56 I=1,NZ
65*              P12(I) = BIJK*BJ(I) + XNE*OM12
66*              P21(I) = BIJK*BJ(I) + AP + XNE*OMEGA
67*          56 CONTINUE
68*          61 DO 66 I=1,NZ
69*              PN = P21(I) + P2K
70*              PB = (P12(I)*P2K)/PN
71*              PA = (P21(I)*PK2*(XEK/XE1))/PN
72*              EB(I) = (C1K + PB)/RS
73*              EA(I) = (C1K + PA)/RS
74*          66 CONTINUE
75*          DO 71 I=1,NZ
76*              XN1(I) = XNT/(1.0 + R1(I) + RK(I))
77*              XN2(I) = R1(I)*XN1(I)
78*              XNK(I) = RK(I)*XN1(I)
79*              ZKL(I) = CP*XN1(I)
80*          71 CONTINUE
81*              ZTL = 1.000001*ZT
82*              ZL = ALOG10(ZTL)
83*              KL = ZL
84*              LL = KL - ND
85*              Z(1) = 0.0
86*              Z(2) = 10.0**LL

```

```

87*
88*
89*
90*
91*      Z(3) = 2.0*Z(2)
92*      Z(4) = 5.0*Z(2)
93*      NDH = 3*ND + 1
94*      NDHP = NDH + 1
95*      IF (ND.EQ.1) GO TO 81
96*      DO 76 I=5,NDH
97*      Z(I) = 10.0*Z(I-3)
98*
99*      76 CONTINUE
100*      81 DO 86 J=NDHP,NZ
101*          JJ = NZ - J + 1
102*          Z(J) = ZT - Z(JJ)
103*      86 CONTINUE
104*          ST = 0.0
105*          T(I) = Z(I)
106*          DO 91 I=2,NZ
107*              DZ = Z(I) - Z(I-1)
108*              T(I) = ST + 0.5*DZ*(ZKL(I-1) + ZKL(I))
109*              ST = T(I)
110*      91 CONTINUE
111*      WRITE (6,96)(T(J),J=1,NZ)
112*      96 FORMAT(4H0TAU/(1PD30.18))
113*      WRITE (6,101)
114*      101 FORMAT(18H18OUND = FREE CASE,10X,24HTWO LEVELS AND CONTINUUM)
115*      WRITE (6,106)DA,ND,ZT,XNT
116*      106 FORMAT(11H0INPUT DATA,100X,A6,A3//20H NUMBER OF DECADES =I3/18H GE
117*      10METRIC DEPTH =1PE8.1/18H TOTAL PARTICLES =E11.4)
118*      WRITE(6,111) CP,DY
119*      111 FORMAT(5H CP =1PE11.4/5H DY =E8.1)
120*      WRITE (6,116)BIJK,BIKJ,ENU
121*      116 FORMAT(7H BIJK =1PE11.4/7H BIKJ =E11.4/6H NUK =F12.5)
122*      WRITE (6,121)TCUT
123*      121 FORMAT(7H TCUT =F6.1)
124*      WRITE (6,126)(Z(I),R1(I),RK(I),XN1(I)*XN2(I),XNK(I)*ZKL(I),T(I)*I=
125*      11,NZ)
126*      126 FORMAT(1H0,8X,1HZ,13X,5HN2/N1,10X,5HNK/N1,11X,2HN1,13X,2HN2,13X,2H
127*      1NK,12X,5HKAPPA,11X,3HTAU//(1P8E15.4))
128*      WRITE (6,136)TE,XNE,OM12,OMEGA,OB,OBAR,DBAR,RS,ABAR,RR12,BB,AP,ALP
129*      1HA,BETA
130*      WRITE (6,131)TH
131*      131 FORMAT(8H THETA =1PE19.4)
132*      WRITE(6,132) CON
133*      132 FORMAT(11H0CONSTANT =1PE16.4)
134*      WRITE (6,141)XE1,XE2,XEK
135*      136 FORMAT(5H1TE =1PE22.1/5H NE =E22.4/13H OMEGA(1,2) =E14.4/13H OMEGA
136*      1(2,1) =E14.4/13H OBAR(1,K) =E14.4/13H OBAR(2,K) =E14.4/14H OB-DBA
137*      2R(K,2) =E13.4/13H A-BAR(1,K) =E14.4,5H (TE)/13H A-BAR(2,K) =E14.4/
138*      313H B-BAR(1,2) =E14.4/13H B-BAR(2,1) =E14.4/15H A-PRIME(2,1) =E12.
139*      44/13H ALPHA(K,2) =E14.4/12H BETA(K,2) =E15.4)
140*      141 FORMAT(6H0N1* =1PE21.7/6H N2* =E21.7/6H NKK =E21.7)
141*      WRITE (6,146)(Z(I),BJ(I),EA(I),EB(I),I=1,NZ)
142*      146 FORMAT(1H0,12X,1HZ,19X,1HJ,18X,2HEA,18X,2HEB//(1P4F20.7))
143*          NT = NZ
144*          NTM = NT - 1
145*          READ (5,16)YA,YR
146*          EY = 1.0/3.0
147*          YMAX = T(NT)**EY
148*          JY = (YMAX - 1.0)/DY
149*          NY = JY + 2

```

```

145*      Y(I) = 1.0
146*      DO 166 J=2,NY
147*      YJ = J - 1
148*      Y(J) = Y(I) + YJ*DY
149*      166 CONTINUE
150*      DO 171 I=1,NY
151*      DO 171 J=1,NY
152*      FY(I,J) = 0.0
153*      FIY(I,J) = 0.0
154*      171 CONTINUE
155*      DO 176 I=1,NY
156*      FY(I,I) = 1.0
157*      FIY(I,I) = 1.0
158*      176 CONTINUE
159*      DO 181 J=2,NY
160*      JM = J - 1
161*      DO 181 I=1,JM
162*      YY = (Y(I) - 1.0)/(Y(J) - 1.0)
163*      FY(I,J) = (1.0 - YY)*(1.0 - YB*YY)
164*      FIY(I,J) = FY(I,J)
165*      181 CONTINUE
166*      IE = NOSONIC(FIY,X,NY,LMAX)
167*      IF (IE,EQ,0) GO TO 486
168*      GY(I) = Y(NY) - 1.0
169*      DO 186 J=2,NY
170*      GY(J) = 0.5*(Y(J) - 1.0)*(1.0 - YB/3.0)
171*      186 CONTINUE
172*      DO 191 K=1,NY
173*      AY(K) = 0.0
174*      DO 191 J=1,NY
175*      AY(K) = AY(K) + GY(J)*FIY(J,K)
176*      191 CONTINUE
177*      WRITE (6,196)(Y(I),GY(I),AY(I),I=1,NY)
178*      196 FORMAT(1H0,11X,1HY,18X,2HGP,18X,2HAY/(1P3E20.8))
179*      R = 0.0
180*      DO 201 I=1,NY
181*      EX = Y(I)*TH
182*      RP(I) = AY(I)*EXP(-EX)/Y(I)
183*      R = R + RP(I)
184*      201 CONTINUE
185*      WRITE (6,206)(RP(J),J=1,NY),R
186*      206 FORMAT(3H0RP//(1PE20.7))
187*      WRITE (6,211)
188*      211 FORMAT(6H0FP(Y))
189*      DO 216 I=1,NY
190*      WRITE (6,26)I,(FY(I,J),J=1,NY)
191*      216 CONTINUE
192*      WRITE (6,221)
193*      221 FORMAT(11H0FP INVERSE)
194*      DO 226 I=1,NY
195*      WRITE (6,26)I,(FIY(I,J),J=1,NY)
196*      226 CONTINUE
197*      DO 231 I=1,NY
198*      DO 231 J=1,NY
199*      EF(I,J) = 0.0
200*      DO 231 K=1,NY
201*      EF(I,J) = EF(I,J) + FY(I,K)*FIY(K,J)
202*      231 CONTINUE

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203*      WRITE (6,31)
204*      DO 236 I=1,NY
205*      WRITE (6,26)I,(EF(I,J),J=1,NY)
206* 236 CONTINUE
207*      NTK = NZ
208*      NTKM = NTK - 1
209*      DO 241 M=1,NY
210*      Y3 = Y**3
211*      DO 241 L=1,NTK
212*      TK(L,M) = T(L)/Y3
213* 241 CONTINUE
214*      DO 246 I=1,NZ
215*      IS = I
216*      IF (T(I)=0.5) 246,246,251
217* 246 CONTINUE
218*      ISM = IS
219*      GO TO 256
220* 251 CONTINUE
221*      ISM = IS - 1
222* 256 CONTINUE
223*      KN = 1
224* C          OUTER LOOP ON FREQUENCY --- INDEX K
225*      DO 416 K=1,NY
226*      KK = K
227*      DO 225 I=1,NZ
228*      T(I) = TK(I,K)
229* 225 CONTINUE
230*      NTK = NZ
231*      NTKM = NTK - 1
232*      WRITE (6,271)Y(K)
233* 271 FORMAT(4H1Y =F6.2)
234*      WRITE (6,276)(TK(I,K),I=1,NTK)
235* 276 FORMAT(1H0,11X,2HTK//(1PE20.7))
236*      CALL WMAT(NZ,TCUT)
237*      DO 240 I=1,NTK
238*      DO 240 J=1,NTK
239*      WKLM(I,J) = WLM(I,J)
240*      WKL(I,J) = WL(I,J)
241* 240 CONTINUE
242* 245 CONTINUE
243*      DO 401 I=1,NZ
244*      DO 401 J=1,NZ
245*      SW(I+J) = SW(I+J) + WKLM(I,J)*RP(K)
246*      WP(I+J) = WP(I,J) + CON*RP(K)*WKL(I,J)
247* 401 CONTINUE
248*      WRITE (6,406)
249* 406 FORMAT(17H0WIJK(LAMBDA = 1))
250*      DO 411 I=1,NTK
251*      WRITE (6,26)I,(WKLM(I,J),J=1,NTK)
252* 411 CONTINUE
253* 416 CONTINUE
254*      WRITE (6,421)
255* 421 FORMAT(7H0S(I,J))
256*      DO 426 I=1,NTK
257*      WRITE (6,26)I,(SW(I,J),J=1,NTK)
258* 426 CONTINUE
259*      WRITE (6,427)
260* 427 FORMAT(8H0WP(I,J))

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```

261*      DD 428 I = 1:NTK
262*      WRITE(6,26) I*(WP(I,J),J=1,NTK)
263*      428 CONTINUE
264*      NTKP = NTK + 1
265*      DO 436 I=1,NTK
266*      DO 431 J=1,NTK
267*      EM(I,J) = -SW(I,J)/(R*EA(I))
268*      IF(I,EQ,J) EM(I,J) = EM(I,J) + 1.0
269*      431 CONTINUE
270*      EM(I,NTKP) = EB(I)/EA(I)
271*      436 CONTINUE
272*      WRITE (6,441)
273*      441 FORMAT(7H0M(I,J))
274*      DO 446 I=1,NTK
275*      WRITE (6,26)I*(EM(I,J),J=1,NTKP)
276*      446 CONTINUE
277*      N = NTK
278*      MC = NTKP
279*      V(1) = 4
280*      CALL GJR(EM,NC,NR,N,MC,$476,JC,V)
281*      WRITE (6,451)(EM(I,NTKP),I=1,NTK)
282*      451 FORMAT(4H01/B//(1PE20.7))
283*      DO 456 I=1,NTK
284*      PN = P21(I) + P2K
285*      B(I) = 1.0/EM(I,NTKP)
286*      RK(I) = XE1*X(B(I))
287*      R1(I) = (P12(I) + RK(I)*PK2)/PN
288*      456 CONTINUE
289*      DO 457 I = 1:NTK
290*      RA(I) = 0.0
291*      DO 457 J = 1,NTK
292*      RA(I) = RA(I) + WP(I,J)/B(J)
293*      457 CONTINUE
294*      WRITE(6,461) (Z(I),B(I)+R1(I)+RK(I),RA(I),I=1,NTK)
295*      461 FORMAT(1H0,13X,1HZ,19X+1HB,17X,5HN2/N1,15X,5HNK/N1,16X,3HR1K//(1PS
296*      1E20.4))
297*      PUNCH 466,(R1(J),J=1,NTK)
298*      PUNCH 466,(RK(J),J=1,NTK)
299*      PUNCH 466,(RA(J),J=1,NTK)
300*      466 FORMAT(5E15.8)
301*      471 CALL EXIT
302*      476 WRITE (6,481)
303*      481 FORMAT(21H0ERROR IN EQ. SOLVING)
304*      GO TO 471
305*      486 WRITE (6,491)IE,NY
306*      491 FORMAT(1SH0ERROR IN FP(Y)/5H IE =I3,5X+4HNY =I3)
307*      WRITE (6,211)
308*      DO 496 I=1,NT
309*      WRITE (6,26)I*(FY(I,J),J=1,NT)
310*      496 CONTINUE
311*      GO TO 471
312*      END

```

DIAGNOSTICS

ION TIME = 5.63 CPU SECONDS

```

1*      SUBROUTINE WMAT(NZ,TCUT)
2*      C          CALCULATES W(LAMBDA) AND W(LAMBDA = 1) AT LINE CENTER
3*      DOUBLE PRECISION T,E1,E2,E3,E4,A1,A2,A3,A4,A5,ESB,P1,B2,B3
4*      DOUBLE PRECISION F,FI,XK
5*      COMMON/BLK1/T(31),E1(31),E2(31),E3(31),E4(31)
6*      COMMON/BLK2/F(31,31),FI(31,31),WL(31,31),WLM(31,31),XK(31,31),
7*           XL(31,31)
8*      10 FORMAT(1H0,I4,2X,1P5E20.7/(7X,5E20.7))
9*      NT = NZ
10*     DO 15 I=1,NZ
11*     DO 15 J=1,NZ
12*     WL(I,J) = 0.0
13*     WLM(I,J) = 0.0
14* 15 CONTINUE
15*     NM = NZ - 1
16*     DO 25 I=1,NM
17*     JP = I + 1
18*     DO 20 J=JP,NM
19*     A1 = DABS(T(J-1)-T(I))
20*     IF (A1.GT.TCUT) GO TO 25

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```

21*      A2 = DABS(T(J) - T(I))
22*      A3 = DABS(T(J+1) - T(I))
23*      A4 = T(J) - T(J-1)
24*      A5 = T(J+1) - T(J)
25*      B1 = (T(I)*(ESB(A1,2) - ESB(A2,2)) + DEXP(-A1) - DEXP(-A2)
26*      1 + ESB(A2,3) - ESB(A1,3))/A4
27*      B2 = (T(J-1)/A4)*(ESB(A1,2) - ESB(A2,2)) - (T(J+1)/A5)*(ESB(A2,2)
28*      1 - ESB(A3,2))
29*      B3 = (T(I)*(ESB(A2,2) - ESB(A3,2)) + DEXP(-A2) - DEXP(-A3)
30*      1 + ESB(A3,3) - ESB(A2,3))/A5
31*      WL(I,J) = 0.5*(B1 + B2 + B3)
32*      WLM(I,J) = WL(I,J)
33* 20 CONTINUE
34* 25 CONTINUE
35*      DO 35 J=2,NM
36*      IP = J + 1
37*      DO 30 I=IP,NZ
38*      A3 = DABS(T(I) - T(J+1))
39*      IF (A3.GT.TCUT) GO TO 35
40*      A1 = DABS(T(I) - T(J-1))
41*      A2 = DABS(T(I) - T(J))
42*      A4 = T(J) - T(J-1)
43*      A5 = T(J+1) - T(J)
44*      B1 = (A1/A4)*(ESB(A2,2) - ESB(A1,2)) + ((T(J+1) - T(I))/A5)*(
45*      1 ESB(A3,2) - ESB(A2,2))
46*      B2 = (DEXP(-A3) - DEXP(-A2) + ESB(A2,3) - ESB(A3,3))/A5
47*      B3 = (DEXP(-A2) - DEXP(-A1) + ESB(A1,3) - ESB(A2,3))/A4
48*      WL(I,J) = 0.5*(B1 + B2 + B3)
49*      WLM(I,J) = WL(I,J)
50* 30 CONTINUE
51* 35 CONTINUE
52*      DO 40 I=2,NM
53*      A1 = T(I) - T(I-1)
54*      A2 = T(I+1) - T(I)
55*      B1 = 2.0 - ESB(A1,2) - ESB(A2,2)
56*      B2 = (0.5 - DEXP(-A1) + ESB(A1,3))/A1
57*      B3 = (0.5 - DEXP(-A2) + ESB(A2,3))/A2
58*      WL(I,I) = 0.5*(B1 + B2 + B3)
59*      WLM(I,I) = WL(I,I) - 1.0
60* 40 CONTINUE
61*      DO 45 I=1,NM
62*      A1 = DABS(T(NM)-T(I))
63*      IF (A1.GT.TCUT) GO TO 45
64*      A2 = DABS(T(NZ) - T(I))
65*      A3 = T(NZ) - T(NM)
66*      B1 = (T(I)*(ESB(A1,2) - ESB(A2,2)) + DEXP(-A1) - DEXP(-A2)
67*      1 + ESB(A2,3) - ESB(A1,3))/A3
68*      B2 = (T(NM)/A3)*(ESB(A1,2) - ESB(A2,2))
69*      WL(I,NZ) = B1 - B2
70*      WLM(I,NZ) = WL(I,NZ)
71* 45 CONTINUE
72*      A3 = T(2) - T(1)
73*      DO 50 I=2,NZ
74*      A2 = DABS(T(2) - T(I))
75*      IF (A2.GT.TCUT) GO TO 50
76*      A1 = DABS(T(1) - T(I))
77*      B1 = ((T(2) - T(I))/A3)*(ESB(A2,2) - ESB(A1,2))
78*      B2 = (DEXP(-A2) - DEXP(-A1) + ESB(A1,3) - ESB(A2,3))/A3

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```

79*      WL(I,1) = 0.5*(B1 + B2)
80*      WLM(I,1) = WL(I,1)
81*      50 CONTINUE
82*      IF (A3.GT.TCUT) GO TO 55
83*      WL(I,1) = 0.5*(1.0 - ESB(A3,2) - (0.5 - DEXP(-A3) + ESB(A3,3))/A3)
84*      GO TO 60
85*      55 WL(I,1) = 0.5 - (0.25/A3)
86*      60 WLM(I,1) = WL(I,1) - 1.0
87*      A1 = T(NZ) - T(NM)
88*      IF (A1.GT.TCUT) GO TO 65
89*      WL(NZ,NZ) = 0.5*(1.0 - ESB(A1,2) - (0.5 - DEXP(-A1) + ESB(A1,3))
90*      1 /A1)
91*      GO TO 70
92*      65 WL(NZ,NZ) = 0.5 - (0.25/A1)
93*      70 WLM(NZ,NZ) = WL(NZ,NZ) - 1.0
94*      WRITE (6,75)
95*      75 FORMAT(10H0W(LAMBDA))
96*      DO 80 I=1,NT
97*      WRITE (6,10)I,(WL(I,J),J=1,NT)
98*      80 CONTINUE
99*      WRITE (6,85)
100*     85 FORMAT(14H0W(LAMBDA = 1))
101*     DO 90 I=1,NT
102*     WRITE (6,10)I,(WLM(I,J),J=1,NT)
103*     90 CONTINUE
104*      RETURN
105*      END

```

AGNOSTICS

ION TIME = 2.60 CPU SECONDS

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1* SUBROUTINE GJR(A,NC,NR,N,MC,S,JC,V)
2* DOUBLE PRECISION A,X,V
3* DIMENSION A(NR,NC),JC(1),V(2)
4* C
5* C           JC IS THE PERMUTATION VECTOR
6* C           KD IS THE OPTION KEY FOR DETERMINANT EVALUATION
7* C           KI IS THE OPTION KEY FOR MATRIX INVERSION
8* C           L IS THE COLUMN CONTROL FOR AX=B
9* C           M IS THE COLUMN CONTROL FOR MATRIX INVERSION
10* C
11* C           INITIALIZATION
12* C
13* C           IW=V(1)
14* C           M=1
15* C           S=1.
16* C           L=N+(MC-N)*(IW/4)
17* C           KD=2-MOD(IW/2,2)
18* C           IF(KD.EQ.1) V(2)=0.
19* C           KI=2-MOD(IW,2)
20* C           GO TO (10,20),KI
21* C
22* C           INITIALIZE JC FOR INVERSION
23* C
24* C           10 DO 15 I=1,N
25* C           15 JC(I)=I

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) 6* C -----
) 7* C SEARCH FOR PIVOT ROW
) 8* C -----
29* 20 DO 85 I=1,N
30* GO TO (30+25),KI
31* 25 M=I
32* 30 IF (I.EQ.N) GO TO 55
33* X=-1.
34* DO 35 J=I,N
35* IF (X.GT.ABS(A(J,I))) GO TO 35
36* X = DABS(A(J,I))
37* K=J
38* 35 CONTINUE
39* IF (K.EQ.I) GO TO 55
40* S=-S
41* V(1)=-V(1)
42* GO TO (40+45),KI
43* 40 MU=JC(I)
44* JC(I)=JC(K)
45* JC(K)=MU
46* C -----
47* C INTERCHANGE ROW I AND ROW K
48* C -----
49* 45 DO 50 J=M,L
50* X=A(I,J)
51* A(I,J)=A(K,J)
52* 50 A(K,J)=X
53* C -----
54* C TEST FOR SINGULARITY
55* C -----
56* 55 IF (DABS(A(I,I)).GT.0.0) GO TO 60
57* C -----
58* C MATRIX IS SINGULAR
59* C -----
60* IF (KD.EQ.1) V(1)=0.
61* JC(1)=I=1
62* RETURN 6
63* 60 GO TO (65,70),KD
64* C -----
65* C COMPUTE THE DETERMINANT
66* C -----
67* 65 IF (A(I,I).LT.0.) S=-S
68* V(2) = V(2) + DLOG(DABS(A(I,I)))
69* 70 X=A(I,I)
70* A(I,I)=1.
71* C -----
72* C REDUCTION OF THE I-TH ROW
73* C -----
74* DO 75 J=M,L
75* A(I,J)=A(I,J)/X
76* C -----
77* C TEST OVERFLOW SWITCH. IF ON
78* C RETURN NEGATIVE VALUE OF I IN JC(1)
79* C -----
80* CALL OVERFL (IFL)
81* IF (IFL.EQ.1) GO TO 120
82* 75 CONTINUE
83* C -----

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84*   C      REDUCTION OF ALL REMAINING ROWS
85*   C
86*   DO 85 K=1,N
87*   IF (K.EQ.I) GO TO 85
88*   X=A(K,I)
89*   A(K,I)=0,
90*   DO 80 J=M,L
91*   A(K,J)=A(K,J)-X*A(I,J)
92*   C
93*   C      TEST OVERFLOW SWITCH. IF ON
94*   C      RETURN NEGATIVE VALUE OF I IN JC(1)
95*   C
96*   C      CALL OVERFL (IFL)
97*   C      IF (IFL.EQ.1) GO TO 120
98*   80 CONTINUE
99*   85 CONTINUE
100*  C
101*  C      AX=B AND DET.(A) ARE NOW COMPUTED
102*  C
103*  GO TO (90,115),KI
104*  C
105*  C      PERMUTATION OF THE COLUMNS FOR MATRIX INVERSION
106*  C
107*  90 DO 110 J=1,N
108*  IF (JC(J).EQ.J) GO To 110
109*  JJ=J+1
110*  DO 95 I=JJ,N
111*  IF (JC(I).EQ.J) GO To 100
112*  95 CONTINUE
113*  100 JC(I)=JC(J)
114*  DO 105 K=1,N
115*  X=A(K,I)
116*  A(K,I)=A(K,J)
117*  105 A(K,J)=X
118*  110 CONTINUE
119*  115 JC(1)=N
120*  IF(KD.EQ.1) V(1)=S
121*  RETURN
122*  120 JC(1)=I-I
123*  IF(KD.EQ.1) V(1)=S
124*  RETURN 6
125*  END

```

DIAGNOSTICS

TION TIME = 1.96 CPU SECONDS

```

1*      DOUBLE PRECISION FUNCTION NOSONI(A,X,L,LMAX)
2*      DOUBLE PRECISION A,X,F
3*      DIMENSION A(1),X(1)
4*      N = L = 1
5*      MAX = N*LMAX + L
6*      MAX = N*LMAX + L
7*      DO 10 I=1,L
8*      X(I) = 1.0
9* 10 CONTINUE
10*      K1 = -LMAX
11*      DO 55 K=1,L
12*      K1 = K1 + LMAX
13*      K2 = K1 + K
14*      IF (A(K2)) 15,80,15
15* 15 DO 30 I=1,L
16*      J1 = K1 + I
17*      IF (A(J1)) 20,30,20
18* 20 F = 1.0/A(J1)
19*      X(I) = X(I)*F
20*      DO 25 J1=I,MAX,LMAX
21*      A(J1) = A(J1)*F
22* 25 CONTINUE
23* 30 CONTINUE
24*      A(K2) = X(K)
25*      X(K) = 1.0
26*      DO 50 I=1,L
27*      K1 = K - I
28*      IF (K1) 35,50,35
29* 35 J1 = K1 + I
30*      IF (A(J1)) 40,50,40
31* 40 A(J1) = 0.0
32*      DO 45 J2=I,MAX,LMAX
33*      J1 = J2 + K1
34*      A(J2) = A(J2) - A(J1)

```

```
35*      45 CONTINUE
36*      50 CONTINUE
37*      55 CONTINUE
38*      DO 70 I=1,N
39*      IF (X(I)) 60,80,60
40*      60 F = 1.0/X(I)
41*      DO 65 J1=I,MAX,LMAX
42*      A(J1) = A(J1)*F
43*      65 CONTINUE
44*      70 CONTINUE
45*      NDSOJI = 1
46*      75 RETURN
47*      80 NDSOJI = 0
48*      GO TO 75
49*      END
```

AGNOSTICS

ION TIME = .98 CPU SECONDS

```

1*      DOUBLE PRECISION FUNCTION ESB(X,N)
2*      C          CALCULATES E2, E3, E4, FROM E1
3*      DOUBLE PRECISION X
4*      DOUBLE PRECISION EXIN
5*      IF (X.LE.0.0) GO TO 35
6*      E = EXIN(X)
7*      GO TO (25+10+10,10)*N
8*      10 EX = DEXP(-X)
9*      E = EX + X*E
10*     GO TO (25+25+15,15)*N
11*     15 E = 0.5*(EX - X*E)
12*     GO TO (25+25+25,20)*N
13*     20 E = (EX - X*E)/3.0
14*     25 ESB = E
15*     30 RETURN
16*     35 GO TO (40+45+50,55)*N
17*     40 ESB = 0.0
18*     GO TO 30
19*     45 ESB = 1.0
20*     GO TO 30
21*     50 ESB = 0.5
22*     GO TO 30
23*     55 ESB = 1.0/3.0
24*     GO TO 30
25*     END

```

DIAGNOSTICS

UTION TIME = .46 CPU SECONDS

```

1*      DOUBLE PRECISION FUNCTION EXIN(Y)
2*      C          CALCULATES E;
3*      DOUBLE PRECISION Y
4*      DOUBLE PRECISION X,A,B,C,E,BB,CC
5*      DIMENSION A(6),B(4),C(4)
6*      DATA A/-5.772156D+01,9.9999193D+01,-2.4991055D+01,5.519968D+02,
7*           -9.76004D+03,1.07857D+03/
8*      DATA B/8.5733287401D+00,1.80590169730D+01,8.6347608925D+00,
9*           12.677737343D+01/
10*     DATA C/9.5733223454D+00,2.56329561486D+01,2.10996530827D+01,
11*           13.9584969228D+00/
12*     X = Y
13*     IF (X=1.0) 10,15,15
14* 10  E = A(1) + X*(A(2) + X*(A(3) + X*(A(4) + X*(A(5) + X*A(6))))))
15*     E = E - DLOG(X)
16*     EXIN = E
17*     RETURN
18* 15  BB = B(4) + X*(B(3) + X*(B(2) + X*(B(1) + X)))
19*     CC = C(4) + X*(C(3) + X*(C(2) + X*(C(1) + X)))
20*     E = (BB/CC)*DEXP(-X)/X
21*     EXIN = E
22*     RETURN
23*     END

```

AGNOSTICS

ION TIME = .48 CPU SECONDS

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024-08/30-23:04
6 REL

```

1*      DOUBLE PRECISION FUNCTION ESB(X,N)
2*          CALCULATES E2, E3, E4, FROM E1
3*          DOUBLE PRECISION X
4*          DOUBLE PRECISION EXIN
5*          IF (X.LE.0.0) GO TO 35
6*          E = EXIN(X)
7*          GO TO (25,10,10,10),N
8* 10 EX = DEXP(-X)
9*          E = EX = X*E
10*         GO TO (25,25,15,15),N
11* 15 E = 0.5*(EX = X*E)
12*         GO TO (25,25,25,20),N
13* 20 E = (EX = X*E)/3.0
14* 25 ESB = E
15* 30 RETURN
16* 35 GO TO (40,45,50,55),N
17* 40 ESB = 0.0
18*         GO TO 30
19* 45 ESB = 1.0
20*         GO TO 30
21* 50 ESB = 0.5
22*         GO TO 30
23* 55 ESB = 1.0/3.0
24*         GO TO 30
25* END

```

DIAGNOSTICS

ATION TIME = .41 CPU SECONDS

```

1*      DOUBLE PRECISION FUNCTION EXIN(Y)
2*          CALCULATES E1
3*          DOUBLE PRECISION Y
4*          DOUBLE PRECISION X,A,B,C,E,BB,CC
5*          DIMENSION A(6),B(4),C(4)
6*          DATA A/-5.772156D=01,9.9999193D=01,-2.4991055D=01,5.519968D=02,
7*          1-9.76004D=03,1.07857D=03/
8*          DATA B/8.5733287401D+00+1.80590169730D+01+8.6347608925D+00,
9*          12.677737343D=01/
10*          DATA C/9.5733223454D+00+2.56329561486D+01+2.10996530827D+01,
11*          13.9584969228D+00/
12*          X = Y
13*          IF (X=1.0) 10,15,15
14* 10 E = A(1) + X*(A(2) + X*(A(3) + X*(A(4) + X*(A(5) + X*A(6)))))
15*          E = E - DLOG(X)
16*          EXIN = E
17*          RETURN
18* 15 BB = B(4) + X*(B(3) + X*(B(2) + X*(B(1) + X)))
19*          CC = C(4) + X*(C(3) + X*(C(2) + X*(C(1) + X)))
20*          E = (BB/CC)*DEXP(-X)/X
21*          EXIN = E
22*          RETURN
23* END

```

IAGNOSTICS

TION TIME = .44 CPU SECONDS